PNNL-15640

Pacific Northwest
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Screening Values for Non-Carcinogenic Hanford Waste Tank Vapor Chemicals that Lack Established Occupational Exposure Limits

TS Poet
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February 2006

Prepared for the U.S. Department of Energy
under Contract DE-AC05-76RL01830

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Richland, Washington 99352

Executive Summary

Over 1,500 different volatile chemicals have been reported in the headspaces of tanks used to store high-level radioactive waste at the U.S. Department of Energy's Hanford Site. Concern about potential exposure of tank farm workers to these chemicals has prompted efforts to evaluate their toxicity, identify chemicals that pose the greatest risk, and incorporate that information into the tank farms industrial hygiene worker protection program. Using occupational exposure limits (OELs) established by U.S. governmental and non-governmental agencies, 52 chemicals of potential concern were previously identified, and an extensive industrial hygiene monitoring program was launched to evaluate these chemicals in the workers' breathing zone. However, approximately 1,400 of the headspace chemicals do not have established OELs. This report identifies which of those headspace chemicals should be further assessed for their potential health risks to tank farm workers.

Headspace concentration screening values were established for each chemical using available industrial hygiene and toxicological data. Screening values were intended to be more than an order of magnitude below concentrations that may cause adverse health effects in workers, assuming a 40-hour/week occupational exposure. Screening values were compared to the maximum reported headspace concentrations.

Approximately 700 of the headspace chemicals lacking established OELs are hydrocarbons that include straight, branched, and cyclic alkanes and alkenes; a small number of alkynes; and a small number of aromatic compounds. This report only addresses worker exposure hazards associated with high-boiling hydrocarbons; those associated with lower-boiling hydrocarbons were considered by Mackerer (2005). None of the chemicals considered is a known or probable human carcinogen as defined by the U.S. Environmental Protection Agency or International Agency (IARC) for Research on Cancer; however; six chemicals considered as possible carcinogens (IARC classification 2B) were included in this evaluation to determine the need for further assessment.

Screening values were assigned to 606 chemicals. Of these, 72 were determined to have been reported in headspaces at or above their screening values, and 14 of the 72 chemicals were found in 15 or more tanks. However, most of the chemicals identified as needing further analysis were observed in the headspace of five or fewer tanks. For 46 of these chemicals, little or no toxicology information was found. Lack of toxicological data specific to the chemical of interest was not considered grounds for assuming the chemical was either toxic or non-toxic at low concentrations in this screening process, and a weight-of-evidence approach was used based on similarities to other chemicals and general principles of toxicology. For chemicals that had little or no toxicological data, data from a surrogate chemical with a more robust toxicology database was used. Using a surrogate chemical with a well-characterized toxicity database resulted in a clearer dose-response relationship. When using surrogates, a greater safety factor was employed.

Over 10% of all of the non-hydrocarbon chemicals identified in the tank waste headspaces were found to be at sufficient levels to warrant further assessment. Of the six possible carcinogens considered, all but acetamide and 1-phenylethanol were identified as needing further analysis. All chemicals for which screening values were developed are listed in the Appendix tables. Any chemicals with a reported maximum concentration that exceeded the screening value will be further evaluated subsequent to this report.

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Tables

Acronyms and Abbreviations

ACGIH	American Conference of Governmental Industrial Hygienists
AIHA	American Industrial Hygienist Association
AOEL	Acceptable Occupational Exposure Limit
CAS	Chemical Abstracts Service
EPA	U.S. Environmental Protection Agency
HSDB®	Hazardous Substances Data Bank
IARC	International Agency for Research on Cancer
LC_{50}	lethal Concentration for 50% of test population
NIOSH	National Institute for Occupational Safety and Health
NLM	National Library of Medicine
NOELs	No-Observed-Effect Levels
OEL(s)	Occupational Exposure Limit(s)
OSHA	Occupational Safety and Health Administration
ppm	parts per million
RTECS®	Registry of Toxic Effects of Chemical Substances
TLV®	threshold limit value (ACGIH-specific)
TOXNET®	The Toxicology Data Network
TWINS	Tank Waste Information Network System

1.0 Introduction

Over 1,500 different volatile chemicals have been reported in the headspaces of tanks used to store high-level radioactive waste at the U.S. Department of Energy Hanford Site (TWINS 2005). Concern about the potential exposure of tank farm workers to these chemicals has prompted efforts to evaluate their toxicity, identify those chemicals that pose the greatest risk to workers, and incorporate that information into the tank farms industrial hygiene worker protection program (Honeyman et al. 2004). Using occupational exposure limits (OELs) established by U.S. governmental and non-governmental agencies, Honeyman et al. (2004) identified 52 chemicals of potential concern, and an extensive industrial hygiene monitoring program has been launched to evaluate these chemicals in the workers' breathing zone. However, roughly 1,400 of the headspace chemicals do not have established OELs and were designated as needing further consideration.

The purpose of this report is to identify those chemicals in the tank waste headspace (lacking established OELs) that should be further assessed for their potential health risks to tank farm workers. This was accomplished by establishing headspace concentration screening values for each chemical using available industrial hygiene and toxicological data. Screening values were intended to be more than an order of magnitude below concentrations that may cause adverse health effects in workers, assuming a 40-hour/week occupational exposure. Screening values were compared to the maximum reported headspace concentrations. Any chemical with a reported maximum concentration that exceeded the screening value will be further evaluated subsequent to this report.

Further analysis of chemicals with screening values below maximum headspace concentrations will include reevaluation of their presence in the tank headspaces to verify chemicals were correctly identified. Chemicals verified to be components of the headspace will then undergo a more detailed toxicological evaluation to develop Acceptable Occupational Exposure Limit (AOEL) guidelines for worker protection (PNNL 2006). Sampling and analytical methods will be developed as necessary and deployed to determine which, if any, of these chemicals are present in the workers' breathing zone and at what concentrations. Based on these additional evaluations, workplace controls will be established as needed by the CH2M HILL Environmental Assessment Strategy Review Group. Chemicals deemed to present no health risks (with maximum headspace concentrations below their screening values) will be listed as low-risk chemicals and reevaluated as new toxicological data become available.

Out of the roughly 1,400 headspace chemicals lacking established OELs, about 700 are hydrocarbons. These hydrocarbons include straight, branched, and cyclic alkanes and alkenes; a small number of alkynes; and a small number of aromatic compounds. Only worker exposure hazards associated with high-boiling hydrocarbons are addressed in this report; those associated with lower-boiling hydrocarbons were considered by Mackerer (2005).

Also, none of the chemicals considered here have established U.S. OELs; these have been addressed by Honeyman et al. (2004).

2.0 Approach

The determination of whether a chemical detected in the tank headspaces is potentially hazardous was based on a comparison of the maximum reported headspace concentration to a screening value. The screening value is the tank headspace vapor concentration above which potential adverse effects of exposures to the workers should be evaluated. Based on criteria developed by Honeyman et al. (2004), screening values are intended to be at least a factor of ten smaller than an 8-hour, time-weighted average OEL. This guideline is conservative for worker protection because:

- The tank headspaces are well isolated from the workers' breathing zone, and headspace concentrations represent source terms at ventilation points.

- Concentrations in the workers' breathing zone are typically many orders of magnitude lower than in the tank headspaces (Hewitt 1996).

- The maximum headspace concentration in a given tank is generally an extreme value and does not represent the typical concentration of a chemical in most tank headspaces (Stock and Huckaby 2004).

- Most reported headspace chemicals have only been detected in a small number of tanks (detection limits for organic vapors have generally been about 0.01 part per million [ppm] or lower), and the probability of exposure to any given chemical is correspondingly less.

3.0 Procedures

This section provides general descriptions of the procedures used to develop the list of headspace chemicals, specify their maximum headspace concentrations, and develop screening values.

3.1 Identified Chemicals and Headspace Concentrations

Headspace characterization data were obtained from the Tank Characterization Database via the Tank Waste Information Network System (TWINS).[(a)] All headspace vapor analysis results for all single-shell and double-shell tanks as well as "stack," "ventilation," and "vent system" were obtained via a TWINS query on July 14, 2005.

Data were eliminated if they were

- marked as suspect (TWINS Vapor Data Qualifier flag S);
- associated with a contaminant in a blank, trip blank, or field blank (TWINS Vapor Data Qualifier flags B, T, or F);
- less than the Vapor Program Required Quantitation Limits (TWINS Vapor Data Qualifier flag Q);
- tentatively identified chemical not detected in the sample (TWINS Vapor Data Qualifier flag M); or
- below the analytical reporting limit (TWINS Vapor Data Qualifier flag U).

Results associated with analytes that were ambiguously identified (e.g., "alkane," "unknown," "C6 ketone") were deleted if the identification was too vague to allow specification of the molecular weight. Results reported as mixtures of analytes were retained if the molecular weight of at least one of the analytes could be unambiguously specified (e.g., "octanenitrile and others" was kept). Mixtures of two or more chemicals (e.g., "acetaldehyde and methanol") were entered separately for each analyte, and each analyte was assumed to be at the reported concentration of the mixture.

The resulting data were averaged by sample device and laboratory for each day of sampling from a given source (tank, vent system, etc.). This process resulted in averaged individual sample results and preserved the distinction between results from different devices (e.g., sorbent traps and SUMMA canisters) and the various analytical laboratories involved. The maximum averaged concentrations were then determined for each tank and ventilation system. The highest average concentrations (from all tanks and ventilation systems) were tabulated. Chemicals with established OELs were identified and removed from the list of chemicals needing screening values.

3.1.1 Headspace Concentration Screening Values

Screening values were developed for each chemical. Data used to develop the screening values were ranked according to relevance to occupational exposure. If no appropriate exposure guidelines for the chemical of interest were identified, an OEL based on a structurally related chemical (surrogate) was

(a) TWINS is available online via the Hanford intranet: http://twins.pnl.gov.

applied. When no OEL for the chemical or a chemical surrogate was available, the assessment was based on identification of toxic effects that were most relevant to occupational exposure. Toxicological parameters were assessed on the basis of metabolic analogies, persistence, chemical and physical properties, chemical structures, and biological activity.

The chemicals were first grouped by chemical class (e.g., alcohols, ketones), sub-grouped as warranted (e.g., alcohols were sub-grouped into alkanols, alkenols, cycloalkanols, etc.), and sorted according to structure (e.g., butanol and alkyl-substituted butanols preceded pentanol and alkyl-substituted pentanols). This grouping simplified the acquisition of toxicological data and facilitated the evaluation of structure-activity relationships. Screening values were then developed for each chemical within a chemical class by a qualified toxicologist and reviewed for accuracy and consistency.

Screening values were assigned to be 10% of a suitable OEL when an established OEL from a non-U.S. agency was available. Additional safety factors were included when a surrogate chemical was used to establish the screening value, when differences between the chemical and chosen surrogate chemical were deemed significant, when the surrogate chosen was based on a metabolite, and when the chemical itself was a possible carcinogen. Screening values could also be raised by a factor of 10 if they had documented low toxicity. The magnitude of the safety factors were based on judgment by the responsible toxicologist and were applied as outlined in Table 1. Default safety factors were usually applied in increments of 10 to ensure conservative estimates. In some cases, factors of 3 were used, based on the judgment of the responsible toxicologist.

Table 1. Screening Factor Values

Comment	Safety Factor
Chemicals without OELs, use of surrogate	Increase (x 10)
Chemicals that are potential carcinogens	Increase (x 10)
Other Factors	
Surrogate structurally different from target chemical	Increase (x 10)
Surrogate/OEL based on surrogate for a metabolite	Increase (x 10)
Chemical with documented low toxicity	Decrease (÷ 10)

Screening values for each chemical were assigned as follows:

1. The publicly available toxicological databases listed in Table 2 were queried for information applicable to toxicological assessment of chemicals. When data were not found in these databases, a broader literature search was conducted. Key toxicological data considered in the specification of the screening value were recorded in a comment field associated with the chemical (see Appendix Tables A.1 through A.15).

Table 2. Toxicological Databases

TOXNET®	The Toxicology Data Network, a set of databases covering toxicology, hazardous chemicals, and related areas; it is maintained by the National Library of Medicine (NLM) (http://toxnet.nlm.nih.gov/).
HSDB®	Hazardous Substances Data Bank. Accessible through TOXNET. Provided by the NLM.
PUBMED®	PubMed, provided by the NLM, contains citations for biomedical articles back to the 1950s; sources include MEDLINE and additional life science journals. (http://www.ncbi.nlm.nih.gov/entrez/query.fcgi?db=PubMed).
RTECS®	Registry of Toxic Effects of Chemical Substances, provided by Thomson Micromedex, Inc., Greenwood Village, Colorado. Accessed through TOMES®, which has the same provider.
TOMES®	Database provided by Thomson-Micromedex, Inc.

2. Non-U.S.-established OELs for the chemical were sought. The primary source for these was *Documentation of the TLVs and BEIs with Other Worldwide Occupational Exposure Values* (ACGIH 2004). OELs established by Canada and European countries were usually considered approximately equivalent to U.S. OELs, but Russian OELs were considered too inconsistent with U.S. OELs and were not used. If a suitable non-U.S. OEL was found for the chemical, it was divided by a safety factor of 10 to obtain the screening value (i.e., used the same as a U.S. regulatory value for screening purposes).

3. If no suitable non-U.S. OEL was found for the chemical, one or more chemical surrogates (i.e., chemicals that are structurally similar and can be expected to have similar toxicological effects) were sought. The selection of surrogates and the evaluation of the toxicological equivalency of surrogates were based on professional judgment. Surrogates generally were of two types:

   Type 1 surrogates had an established U.S. OEL. These were usually obtained from the American Conference of Governmental Industrial Hygienists (ACGIH) (2004), which lists ACGIH threshold limit values (TLV®s) and ceilings, the Occupational Safety and Health Administration (OSHA) permissible exposure limits (PELs), the National Institute for Occupational Safety and Health (NIOSH) recommended exposure limits, American Industrial Hygienist Association (AIHA) workplace environmental exposure levels and exposure limits assigned in foreign countries, if available. ACGIH guideline documentation for the surrogate was reviewed and compared with any toxicological data obtained for the chemical of interest. Depending on the chemical and toxicological similarities of the surrogate to the chemical of interest, the screening value was established by dividing the surrogate OEL by an additional safety factor of 10 or greater, using the guidelines in Table 1.

   Type 2 surrogates did not have an established U.S. OEL but did have toxicological data that could be used to evaluate the chemical of interest. A safety factor of at least 10 was applied for the use of a surrogate, and additional safety factors were applied, as necessary, depending on whether the chemical of interest was deemed to be less or more toxic than the surrogate.

4. If no OEL or satisfactory surrogate was identified, as was the case for a number of chemicals, the toxicologist performed the screening based on experience and general information found in

toxicology texts such as those listed in the bibliography. These cases are noted in the comments column of the tables in the Appendix.

Published information used during this screening effort included any or all of the following:

- Acute lethality data for one or more animal species.
- The lowest dose/concentration at which toxic effects were noted for the referenced species. Inhalation studies are the most desirable.
- Effects of cumulative exposures, which could range from short-term to long-term studies. Inhalation studies are the most desirable.
- If the route of exposure was other than inhalation, efforts should be made to extrapolate to a dose given by inhalation.
- The most desirable studies have a range of doses that demonstrate high to low dose responses.

A summary of the information used is provided in the Appendix tables in the comments column for each chemical. If data from the Hazardous Substances Data Bank (HSDB) and/or Registry of Toxic Effects of Chemical Substances (RTECS) files were considered sufficient, that is stated. In some cases, original research articles were used and are cited.

4.0 Screening Results and Discussion

Chemicals for which screening values were developed are listed in the Appendix tables with their respective Chemical Abstracts Service (CAS) or TWINS identification number. These tables also include primary surrogate(s) used to establish screening values with the surrogate OELs and source of the OEL. Cumulative safety factors applied to the surrogate OEL and the screening value itself are given along with comments. The third column in the tables lists the maximum reported headspace concentration of each chemical. When this value is equal to or greater than the screening value, it is given in bold typeface with a shaded background.

Of the 606 chemicals assigned screening values, 72 were determined to have been reported in headspaces at or above their screening values (see Table 3 and Appendix Table A.16). Fourteen of the 72 chemicals were found in 15 or more tanks. Most of the chemicals identified as needing further analysis, however, were observed in the headspace of five or fewer tanks.

For 46 of these chemicals, little or no toxicology information was found. Lack of toxicological data specific to the chemical of interest was not considered grounds for assuming the chemical was either toxic or non-toxic at low concentrations in this screening process, and a weight-of-evidence approach was used based on similarities to other chemicals and general principles of toxicology. When a chemical had little or no toxicological data, data from a surrogate chemical with a more robust toxicology database were used. The use of a surrogate chemical with a well-characterized toxicity database resulted in a clearer dose-response relationship and defined no-observed-effect levels (NOELs), LC_{50}s, and OELs. However, when utilizing surrogates, greater safety factor was employed. A brief written assessment of the overall strengths and weaknesses of the surrogate chemical is included in the comments column of the tables in the Appendix.

Although this report does not consider known or probable human carcinogens, six of the chemicals considered were listed by IARC as possible carcinogens (IARC 2B), and three utilized structurally similar surrogates that ACGIH has designated as a confirmed animal carcinogen with unknown relevance to humans (A3). NIOSH recommends limiting occupational exposures to carcinogens to the lowest feasible concentration (NIOSH 1997). Screening values included the carcinogenic potential of these compounds, and the safety factors were often 1,000. Further analysis to determine AOELs for these compounds will address the importance of the carcinogenic potentials.

Of the possible carcinogens considered in this report, all but acetamide and 1-phenylethanol were identified by the screening criteria as needing further analysis to determine an AOEL. Because no effects were seen in mice or the kidneys of female rats, it is proposed that 1-phenylethanol not undergo further assessment at this time; however, if more data become available, a more rigorous (AOEL) assessment should be reconsidered. Based on its carcinogenic potential, acetamide should be included on the list of chemicals needing further assessment.

It is recognized that in the course of developing OELs for the chemicals listed in Tables 3 and 4, related chemicals, even when not specifically identified based on screening values, may also be evaluated. For example, substituted furans should be further evaluated as part of the AOEL process since they share a common structure with the parent furan, which suggests that they may likewise be of concern as potential carcinogens.

Table 3. Chemicals with Maximum Headspace Concentrations Greater Than Their Screening Values

	CAS or TWINS Number	Chemical	Max. Conc. (ppm)	Screening Value (ppm)	Number of Tanks
		HALOCARBONS			
1	78-76-2	2-Bromobutane	0.023	0.01	2
2	1184-60-7	2-Fluoropropene	0.53	0.01	5
3	10061-02-6	E-1,3-Dichloropropene	0.010	0.001	7
4	10061-01-5	Z-1,3-Dichloropropene	0.0092	0.001	5
		ALCOHOLS			
5	617-94-7	Phenyl-a,a-dimethylmethanol	2.2	0.1	5
6	36653-82-4	1-Hexadecanol	1.1	0.015	15
7	112-92-5	1-Octadecanol	0.96	0.015	4
8	96-41-3	Cyclopentanol	1.9	0.5	5
9	627-27-0	3-Buten-1-ol	5.7	0.07	3
		ETHERS			
10	628-28-4	1-Methoxybutane	0.43	0.05	3
		ALDEHYDES			
11	1115-11-3	2-Methylbut-2-enal	0.013	0.003	1
12	645-62-5	2-Ethylhex-2-enal	0.028	0.003	2
13	UAD010-01	Decadienal	0.015	0.003	1
		KETONES			
14	105-42-0	4-Methyl-2-hexanone	1.1	0.05	4
15	589-38-8	3-Hexanone	6.3	2	17
16	928-68-7	6-Methyl-2-heptanone	2.1	0.5	30
17	821-55-6	2-Nonanone	1.6	0.05	21
18	1534-27-6	3-Dodecanone	1.1	0.5	13
19	1534-26-5	3-Tridecanone	0.61	0.5	18
20	UKE008-01	C8-Alkanone	1.2	0.5	6
21	UKE009-03	C9-Alkanone	1.1	0.5	1
22	UKE013-02	C13-Alkanone	1.1	0.5	1
23	89-82-7	5-Methyl-2-(1-methylethenyl) cyclohexanone	0.37	0.2	2
24	4176-04-9	4,7,7-Trimethyl bicyclo[4.1.0]heptan-3-one	0.086	0.02	1
25	814-78-8	3-Methyl-3-buten-2-one	0.021	0.002	2
		ACIDS			
26	UCA016-01	C16-Alkanoic acid	1.1	1	1
		ESTERS			
27	1838-59-1	2-Propenyl formate	1.1	1	1
28	74381-40-1	1-(1,1-Dimethylethyl)-2-methyl-1,3-propanediyl 2-methylpropanoate	0.45	0.1	12
29	20474-93-5	2-Propenyl 2-butenoate	0.29	0.15	1
30	110-27-0	1-Methylethyl tetradecanoate	0.17	0.0035	7
31	110-36-1	Butyl tetradecanoate	0.20	0.0035	4
32	142-91-6	1-Methylethyl hexadecanoate	0.033	0.0035	32
33	78-46-6	Dibutyl butylphosphonate	0.070	0.002	7
		NITRILES			
34	1647-11-6	2-Methylene butanenitrile	0.043	0.02	1
35	110-59-8	Pentanenitrile	1.1	0.08	57
36	628-73-9	Hexanenitrile	0.85	0.08	58
37	629-08-3	Heptanenitrile	0.64	0.08	45
38	124-12-9	Octanenitrile	0.49	0.08	22

Table 3. (contd)

	CAS or TWINS Number	Chemical	Max. Conc. (ppm)	Screening Value (ppm)	Number of Tanks
		NITRILES			
39	2243-27-8	Nonanenitrile	0.16	0.08	19
40	1975-78-6	Decanenitrile	0.16	0.08	3
41	109-75-1	3-Butenenitrile	0.021	0.02	2
42	1615-70-9	2,4-Pentadienenitrile	0.041	0.02	2
		AMINES & AMIDES			
43	22431-09-0	N-(1-Methylbutylidene)methanamine	0.13	0.05	5
44	1072-44-2	N-Methylaziridine	0.065	0.02	1
45	2549-67-9	2-Ethylaziridine	0.056	0.02	5
46	616-45-5	2-Pyrrolidinone	0.25	0.1	5
		NITRITES & NITRATES			
47	624-91-9	Methyl nitrite	0.32	0.2	14
48	544-16-1	Butyl nitrite	0.49	0.4	7
49	928-45-0	Butyl nitrate	0.36	0.25	22
50	3457-90-7	1,3-Propanediol, dinitrate	0.018	0.0005	1
51	3457-91-8	1,4-Butanediol, dinitrate	0.26	0.0005	5
52	3457-92-9	1,5-Pentanediol, dinitrate	0.0032	0.0005	4
53	624-43-1	1,2,3-Propanetriol, 1-nitrate	0.026	0.0005	1
54	623-87-0	1,2,3-Propanetriol, 1,3-dinitrate	0.010	0.0005	2
		NITRO COMPOUNDS			
55	2902-96-7	2-Nitro-1-propanol	0.43	0.1	1
56	594-70-7	2-Nitro-2-methylpropane	0.23	0.1	31
57	627-05-4	1-Nitrobutane	0.39	0.25	5
		NITROSO COMPOUNDS			
58	59-89-2	4-Nitrosomorpholine	0.0097	0.005	1
		HETEROCYCLICS			
59	56052-94-9	cis-2-Ethyl-3-propyloxirane	0.030	0.02	1
60	110-00-9	Furan	3.2	0.01	11
61	534-22-5	2-Methylfuran	1.0	0.01	2
62	4229-91-8	2-Propylfuran	0.60	0.01	2
63	1703-52-2	2-Ethyl-5-methylfuran	0.010	0.01	2
64	1708-29-8	2,5-Dihydrofuran	1.8	0.5	5
65	1192-51-4	3-Methyl-2,4(3H,5H)-furandione	0.0035	0.0025	1
66	31681-26-2	α-Propylfuranacetaldehyde	0.030	0.02	1
67	UHC000-09	Methylpyridine	0.52	0.2	3
68	108-47-4	2,4-Dimethylpyridine	0.10	0.1	4
69	694-05-3	1,2,3,6-Tetrahydropyridine	0.093	0.05	4
70	UHC000-13	C2-Pyridine	0.19	0.05	1
		SULFUR COMPOUNDS			
71	UIN000-01	Sulfur oxides (SOx)	0.37	0.02	1
72	3622-84-2	N-Butylbenzenesulfonamide	0.16	0.015	39

The purpose of this toxicological review of waste tank vapors that lack established OELs was to identify all of the chemicals in the headspace for which AOELs are needed to protect worker health. Over 10% of all of the non-hydrocarbon chemicals identified in the tank waste headspaces were found to be at sufficient levels to warrant an assessment of an AOEL (See Table 4). The conservative nature of this screening procedure suggests that AOELs will likely be higher than the screening values that prompted their development.

Table 4. Chemicals Listed as Possible Human Carcinogens

Chemical	Max. Conc. (ppm)	Screening Value (ppm)	Carcinogen Comments
E-1,3-Dichloropropene	0.010	0.001	IARC (1987) classifies 1,3-dichloropropene as 2B, or possible human carcinogen. The lack of human data, the lack of extensive and conclusive animal studies, the capability of 1,3-dichloropropene to cause DNA fragmentation and lesions, the structural similarity to known carcinogens, and mutagenic potential imply that further research is necessary for 1,3-dichloropropene.
Z-1,3-Dichloropropene	0.0092	0.001	IARC (1987) classifies 1,3-dichloropropene as 2B, or possible human carcinogen. The lack of human data, the lack of extensive and conclusive animal studies, the capability of 1,3-dichloropropene to cause DNA fragmentation and lesions, the structural similarity to known carcinogens, and mutagenic potential imply that further research is necessary for 1,3-dichloropropene.
1-Phenylethanol	0.0047	0.01	IARC (1999) classifies 1-phenylethanol as a 2B, or possible human carcinogen - NTP Bioassay via gavage - no tumors in mice, renal tubular adenoma in male rats.
Acetamide	0.0032	0.01	IARC (1999) classifies acetamide as 2B, or possible human carcinogen. Animal studies have reported liver tumors from oral exposure to acetamide (1, 3, 4, and 5). EPA has not classified acetamide for carcinogenicity. The California EPA has established an inhalation unit risk estimate of 2 × 10-5(µg/m3)-1 and an oral cancer slope factor of 7×10^{-2}(mg/kg/d)-1 for acetamide(5)
4-Nitrosomorpholine	0.0097	0.005	IARC (1987) classifies 4-nitrosomorpholine as 2B, or possible human carcinogen. N-Nitrosomorpholine is carcinogenic in mice, rats, hamsters, and various fish. Following oral administration, it produces benign and malignant tumors of the liver and lung in mice; of the liver, kidney, and blood vessels in rats; and of the liver in hamsters. NTP: Suspect Human Carcinogen.
Furan	3.2	0.01	Furan is reasonably anticipated to be a human carcinogen based on evidence of malignant tumor formation at multiple tissue sites in multiple species of experimental animals (IARC 1995) and is classified by IARC as 2B, or possible human carcinogen. Furan was tested for carcinogenicity by oral administration in one study in mice and in one study in rats. It produced hepatocellular adenomas and carcinomas in mice. In rats, it produced hepatocellular adenomas in animals of each gender and carcinomas only in males; a high incidence of cholangiocarcinomas was seen in both males and females. The incidence of mononuclear-cell leukemia was also increased in animals of each gender.
Substituted Furans	0.0008 to 1.8	NA	For the broad range of chemicals containing the unsaturated furan nucleus, experimental evidence suggests that observed toxicity in several target organs involves the formation of a chemically reactive metabolite from a 5-member, oxygen-containing, unsaturated heterocyclic ring. The common toxic moiety suggests that carcinogenicity may also be related in this class of chemicals.

NA = not applicable.

5.0 References

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Appendix

Chemical Screening Values

Appendix

Chemical Screening Values

Acronyms

ACGIH	American Conference of Governmental Industrial Hygienists
CAS	Chemical Abstracts Service
CCRS	Chemical Carcinogenesis Research Information System
CNS	central nervous system
CVS	cardiovascular system
CHO	Chinese hamster ovary
EL	Exposure Limit
HSDB®	Hazardous Substances Data Bank
IARC	International Agency for Research on Cancer
IRIS	Integrated Risk Information System
LC_{50}	lethal Concentration for 50% of test population
LCLo	lowest lethal concentration
LD	lethal dose
LDLo	lowest lethal dose
LD_{50}	lethal dose for 50% of test population
MAC/MAK	Maximum Allowable Concentration (*Maximale Arbeitsplatzkonzentrationen*)
MSDS	Material Safety Data Sheets
MW	molecular weight
NIOSH	National Institute for Occupational Safety and Health
NOEL	no-observed-effect level
OEL	occupational exposure limit
OSHA	Occupational Safety and Health Administration
PEL	permissible exposure limit (OSHA-specific)
PubMed	The National Library of Medicine's online search service
REL	recommended exposure limit (NIOSH-specific)
RTECS®	Registry of Toxic Effects of Chemical Substances
SF	Safety Factor
SIRI	Safety Information Resources Inc.
SRC	Syracuse Research Corporation
STEL	short term exposure limit
TCLo	toxic concentration low
TDLo	lowest toxic dose
TLV	threshold limit value (ACGIH-specific)
TOXNET®	The Toxicology Data Network
TWA	time weighted average
WEEL	Workplace Environmental Exposure Level Guidelines

Table A.1. Hydrocarbons

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALKANES						
3892-00-0	2,6,10-Trimethylpentadecane	n-Nonane	200	TLV	100	2	No specific toxicity information located. A toxicologic study indicates that C13 to C16 alkanes, when aspirated into the lungs, are asphyxiants similar to the C6 to C10 members, but cause death more slowly. /ALKANES/ (Clayton, G. D. and F. E. Clayton (eds.). *Patty's Industrial Hygiene and Toxicology*: Volume 2A, 2B, 2C: *Toxicology*. 3rd Ed. New York: John Wiley Sons, 1981-1982., p. 3193]. Based on TLVs for lower molecular weight hydrocarbons, e.g., nonane (111-84-2), this screening value is conservative.
13475-75-7	8-Hexylpentadecane	n-Nonane	200	TLV	100	2	See comment for 2,6,10-Trimethyl-pentadecane (3892-00-0).
21164-95-4	7,9-Dimethylhexadecane	n-Nonane	200	TLV	100	2	See comment for 2,6,10-Trimethyl-pentadecane (3892-00-0).
638-36-8	2,6,10,14-Tetramethyl-hexadecane	n-Nonane	200	TLV	100	2	See comment for 2,6,10-Trimethyl-pentadecane (3892-00-0).
6418-44-6	3-Methylheptadecane	n-Nonane	200	TLV	100	2	See comment for 2,6,10-Trimethyl-pentadecane (3892-00-0).
20959-33-5	7-Methylheptadecane	n-Nonane	200	TLV	100	2	See comment for 2,6,10-Trimethyl-pentadecane (3892-00-0).
13287-23-5	8-Methylheptadecane	n-Nonane	200	TLV	100	2	See comment for 2,6,10-Trimethyl-pentadecane (3892-00-0).
18344-37-1	2,6,10,14-Tetramethyl-heptadecane	n-Nonane	200	TLV	100	2	See comment for 2,6,10-Trimethyl-pentadecane (3892-00-0).
54833-48-6	2,6,10,15-Tetramethyl-heptadecane	n-Nonane	200	TLV	100	2	See comment for 2,6,10-Trimethyl-pentadecane (3892-00-0).
7225-64-1	9-Octylheptadecane	n-Nonane	200	TLV	100	2	See comment for 2,6,10-Trimethyl-pentadecane (3892-00-0).
593-45-3	Octadecane	n-Nonane	200	TLV	100	2	See comment for 2,6,10-Trimethyl-pentadecane (3892-00-0).
1560-88-9	2-Methyloctadecane	n-Nonane	200	TLV	100	2	See comment for 2,6,10-Trimethyl-pentadecane (3892-00-0).
75163-97-2	2,6-Dimethyloctadecane	n-Nonane	200	TLV	100	2	See comment for 2,6,10-Trimethyl-pentadecane (3892-00-0).
629-92-5	Nonadecane	n-Nonane	200	TLV	100	2	See comment for 2,6,10-Trimethyl-pentadecane (3892-00-0).
13287-24-6	9-Methylnonadecane	n-Nonane	200	TLV	100	2	See comment for 2,6,10-Trimethyl-pentadecane (3892-00-0).
112-95-8	Eicosane	n-Nonane	200	TLV	100	2	See comment for 2,6,10-Trimethyl-pentadecane (3892-00-0).
629-94-7	Heneicosane	n-Nonane	200	TLV	100	2	See comment for 2,6,10-Trimethyl-pentadecane (3892-00-0).
55373-86-9	7-Hexyldocosane	n-Nonane	200	TLV	100	2	See comment for 2,6,10-Trimethyl-pentadecane (3892-00-0).
630-01-3	Hexacosane	n-Nonane	200	TLV	100	2	See comment for 2,6,10-Trimethyl-pentadecane (3892-00-0).
630-02-4	Octacosane	n-Nonane	200	TLV	100	2	See comment for 2,6,10-Trimethyl-pentadecane (3892-00-0).

Table A.1. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	Incompletely Identified Alkanes						
UAK018-01	C18-Alkane	n-Nonane	200	TLV	100	2	See comment for 2,6,10-Trimethyl-pentadecane (3892-00-0).
UAK020-01	C20-Alkane	n-Nonane	200	TLV	100	2	See comment for 2,6,10-Trimethyl-pentadecane (3892-00-0).
	CYCLOALKANES						
55282-34-3	1,3,5,-Trimethyl-2-octadecyl-cyclohexane	Cyclohexane	100	TLV	100	1	Based on surrogate of cyclohexane (110-82-7). Screening Value is conservative in light of the high molecular weight of this compound, whose pulmonary absorption rate will be considerably slower than that for cyclohexane.
	ALKENES						
112-88-9	1-Octadecene	1-Decene	100	WEEL	100	1	Screening value set conservatively based on low toxicity of surrogate hydrocarbon and WEEL for 1-decene (872-05-9), Rat-LD50 Oral 10 gm/kg.
18435-45-5	1-Nonadecene	1-Decene	100	WEEL	100	1	Screening value set conservatively based on low toxicity of surrogate hydrocarbon and WEEL for 1-decene (872-05-9), Rat-LD50 Oral 10 gm/kg.
74685-30-6	E-5-Eicosene	1-Decene	100	WEEL	100	1	Screening value set conservatively based on low toxicity of surrogate hydrocarbon and WEEL for 1-decene (872-05-9), Rat-LD50 Oral 10 gm/kg.
	POLYENES						
59681-06-0	2,6,10,19,23-Pentamethyl-2,6,10,14,18,22-tetracoshexaene	n.a.	n.a.	n.a.	n.a.	5	No specific toxicity information for this alkene. Screening value set conservatively based on low toxicity of higher molecular weight hydrocarbons.
7683-64-9	2,6,10,15,19,23-Hexamethyl-2,6,10,14,18,22-tetracoshexaene	n.a.	n.a.	n.a.	n.a.	5	No specific toxicity information for this alkene. Screening value set conservatively based on low toxicity of higher molecular weight hydrocarbons.
59681-06-0	2,6,10,14,18,22-Tetracosahexaene, 2,6,10,19,23-pentamethyl-, (all-E)-	n.a.	n.a.	n.a.	n.a.	5	No specific toxicity information for this alkene. Screening value set conservatively based on low toxicity of higher molecular weight hydrocarbons.
	ALKYNES						
629-89-0	1-Octadecyne	Propyne	1000	TLV	100	10	No specific toxicity information located for this compound. Screening value based on TLV for propyne (74-99-7).

Table A.1. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALKYLBENZENES						
1083-56-3	bis-1,1'-(1,4-Butanediyl) benzene	Xylenes	100	TLV	100	1	No toxicity information located for this compound. Screening value based on TLV for xylenes (1330-20-7).

Table A.2. Halogenated Compounds

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	HALO ALKANES						
460-13-9	1-Fluoropropane	1,2-Dichloropropane	75	TLV	100	0.75	No toxicity information located. Screening Value based on structural similarity to 1,2-dichloropropane (78-87-5).
753-89-9	1-Chloro-2,2-dimethylpropane	1,2-Dichloropropane	75	TLV	100	0.75	No TLVs or toxicity information located for this compound. Screening Value based TLV for 1,2-dichloropropane (78-87-5).
507-55-1	1,3-Dichloro-1,1,2,2,3-pentafluoropropane	1,1,1,2-Tetrachloro-2,2-difluoroethane	500	TLV	300	1.667	Rat: LC50 - ROUTE: Inhalation; 31660 ppm/4H (RTECS). Screening Value based on structural similarity to 1,1,1,2-Tetrachloro-2,2-difluoroethane (76-11-9) with an additional safety factor of 3 due to structural dissimilarity. Also Chlorodifluoromethane with a NIOSH REL of 1000 ppm
109-69-3	1-Chlorobutane	1,2-Dichloropropane	75	TLV	100	0.75	No TLVs listed; http://docs.appliedbiosystems.com/pebiodocs/00103207.pdf; RTECS Summary: lowest toxic dose-mouse-8,000 ppm for 4 hr; No evidence for carcinogenicity, http://www.cdc.gov/niosh/rtecs/ej602160.html#X. Screening Value based on structural similarity to 1,2-dichloropropane (78-87-5).
78-76-2	2-Bromobutane	Bromomethane	1	TLV	100	0.01	No toxicity information or TLV for this compound; https://fscimage.fishersci.com/msds/97253.htm; Screening Value based on bromomethane (74-83-9).
628-61-5	2-Chlorooctane	Bromomethane	1	TLV	100	0.01	No toxicity information or TLV for this compound; https://fscimage.fishersci.com/msds/97253.htm; Screening Value based on bromomethane (74-83-9).
	HALO ALKENES						
1184-60-7	2-Fluoropropene	Fluoroethene	1	TLV	100	0.01	No toxicity data located. Screening Value assigned on basis of structural similarity to fluoroethene (75-02-5).
10061-02-6	E-1,3-Dichloropropene	3-Chloropropene	1	TLV	1000	0.001	No toxicity information listed in MSDS; however, listed as potential carcinogen, irritant; http://msds.ehs.cornell.edu/msds/siri/files/bwj/bwjfq.html. Screening Value based on structural similarity to 3-chloropropene (107-05-1).

Table A.2. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	HALO ALKENES						
10061-01-5	Z-1,3-Dichloropropene	3-Chloropropene	1	TLV	1000	0.001	No toxicity information listed in MSDS; however, listed as potential carcinogen, irritant; http://msds.ehs.cornell.edu/msds/siri/files/bwj/bwjfq.html. Screening Value based on structural similarity to 3-chloropropene (107-05-1).
	AROMATIC HALOGEN COMPOUNDS						
541-73-1	1,3-Dichlorobenzene	1,2-Dichlorobenzene	25	TLV	100	0.25	No data available for 1,3-dichlorobenzene. Screening Value assigned on basis of structural similarity to 1,2-dichlorobenzene (95-50-1).
	OTHER HALOGENATED COMPOUNDS						
55429-85-1	N-[Perfluorophenyl]-β,4-bis(trimethylsilyloxy) benzeneethanamine	n.a.	n.a.	n.a.	n.a.	1	No information available for this compound. Screening Value set conservatively based on author's experience.
420-56-4	Fluorotrimethylsilane	Chlorotrimethylsilane	5	WEEL Ceiling	100	0.05	No data located for fluorotrimethylsilane. Based on ACGIH OEL for chlorotrimethylsilane (75-77-4).

Table A.3. Alcohols and Phenols

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALKANOLS						
617-94-7	Phenyl-α,α-dimethylmethanol	Phenylmethanol	10	WEEL	100	0.1	Assignment based on structural similarity to phenylmethanol (100-51-6). There is very little information available on either compound; however, what there is gives no indication of unexpected toxicity for this compound; rat, oral LD50 ~2 g/kg; slight indication of human dermal sensitization; mild dermal irritation in guinea pigs and rabbits; mild eye irritation in rabbits (HSDB).
16624-06-9	α,α-Dimethyl cyclooctanemethanol	1-Decanol	n.a.	n.a.	n.a.	0.015	No toxicity information located for this or any closely related compound. Screening Value set conservatively based on other alkyl alcohols, e.g., 1-decanol (112-30-1).
2136-70-1	2-Tetradecyloxyethanol	2-Butoxyethanol	20	TLV	100	0.2	An alkoxy surfactant, used in clean-up of oil spells. No toxicity information located, no MSDS located. Screening Value based on structural similarity to 2-butoxyethanol (111-76-2).
98-85-1	1-Phenylethanol	Phenylmethanol	10	WEEL	1000	0.01	Rat-LD50 - ROUTE: Oral; DOSE: 400 mg/kg; Mouse-LD50 - ROUTE: Subcutaneous; DOSE: 250 mg/kg (RTECS); Some evidence of renal carcinogenicity in rats and mice after 2-yr chronic administration (HSDB). Screening Value based on structural similarity to phenylmethanol (100-51-6).
34386-42-0	4-(1,1-Dimethylethyl)-α-methylbenzenemethanol	Phenylmethanol	10	WEEL	1000	0.01	No toxicity information located for this or closely related compound. Screening Value set conservatively based on other alkyl alcohols, e.g., 1-phenylethanol (98-85-1).
75-84-3	2,2-Dimethyl-1-propanol	2-Methyl-1-propanol	50	TLV	100	0.5	No toxicity information located for this compound. Screening Value based on structural similarity to 2-methyl-1-propanol (78-83-1).
UOH010-01	1-Cyclopentyl-2,2-dimethyl-1-propanol	2-Methyl-1-propanol	50	TLV	100	0.5	No toxicity information located for this or closely related compound. Screening Value set conservatively based on other alkyl alcohols, e.g., 2-methyl-1-propanol (78-83-1).

Table A.3. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALKANOLS						
3944-36-3	1-(1-Methylethoxy)-2-propanol	2-Butoxyethanol	20	TLV	100	0.2	Screening Value based on structural similarity to 2-butoxyethanol (111-76-2).
137-32-6	2-Methyl-1-butanol	3-Methyl-1-butanol	100	TLV	100	1	Screening Value based on structural similarity to 3-methyl-1-butanol (123-51-3).
97-95-0	2-Ethyl-1-butanol	3-Methyl-1-butanol	100	TLV	100	1	Screening Value based on structural similarity to 3-methyl-1-butanol (123-51-3).
624-95-3	3,3-Dimethyl-1-butanol	3-Methyl-1-butanol	100	TLV	100	1	Screening Value based on structural similarity to 3-methyl-1-butanol (123-51-3).
75-85-4	2-Methyl-2-butanol	n.a.	100	Norway TWA	10	10	Rat - TCLo - ROUTE: Inhalation; DOSE: 1500 ppm/6H/7D intermittent (RTECS); OEL-DENMARK: TWA 100 ppm (350 mg/m3), JAN1999 (RTECS). Screening Value based on TCLo and Norway TWA.
54004-41-0	4-Methyl-2-propyl-1-pentanol	4-Methyl-2-pentanol	25	TLV	100	0.25	Assignment based on structural similarity to 4-methyl-2-pentanol (108-11-2).
4799-62-6	5-Methoxy-1-pentanol	1-Methoxy-2-propanol	100	TLV	100	1	Assignment based on structural similarity to 1-methoxy-2-propanol (107-98-2).
71-41-0	1-Pentanol	1-Butanol	20	TLV	100	0.2	Rat and Mouse Lclo- ROUTE: Inhalation; 14000 mg/m3. Iso-amyl alcohol ACGIH TWA TLV 100 ppm.
6032-29-7	2-Pentanol	n.a.	50	Norway TWA	10	5	Set by Norway, no US OEL established. Assignment based on Norwegian TWA.
590-36-3	2-Methyl-2-pentanol	4-Methyl-2-pentanol	25	TLV	100	0.25	Irritant. Assignment based on structural similarity to 4-methyl-2-pentanol (108-11-2).
4911-70-0	2,3-Dimethyl-2-pentanol	4-Methyl-2-pentanol	25	TLV	100	0.25	Irritant. Assignment based on structural similarity to 4-methyl-2-pentanol (108-11-2).
19780-63-3	3-Ethyl-2-methyl-2-pentanol	4-Methyl-2-pentanol	25	TLV	100	0.25	Irritant. Assignment based on structural similarity to 4-methyl-2-pentanol (108-11-2).
565-67-3	2-Methyl-3-pentanol	4-Methyl-2-pentanol	25	TLV	100	0.25	Irritant. Assignment based on structural similarity to 4-methyl-2-pentanol (108-11-2).
3054-92-0	2,3,4-Trimethyl-3-pentanol	4-Methyl-2-pentanol	25	TLV	100	0.25	Irritant. Assignment based on structural similarity to 4-methyl-2-pentanol (108-11-2).

Table A.3. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALKANOLS						
111-27-3	1-Hexanol	1-Pentanol	100	WEEL	100	1	Relatively low tocixity, rat oral LD50 720 mg/kg; mouse 1950 mg/kg. Unlike 2-hexanol, 1-hexanol not known to be a neurotoxicant (HSDB, RTECS). Screening Value based 1-pentanol (71-41-0).
104-76-7	2-Ethyl-1-hexanol	n.a.	50	German MAK	10	5	Screening Value based on German (EU) MAK and similarity to alkyl substituted pentanols.
627-59-8	5-Methyl-2-hexanol	n-Hexane	50	TLV	100	0.5	Very little information on 5-methyl-2-hexanol; however, 2-hexanol, a potential metabolite, can be neurotoxic. 2-hexanol is also a metabolite of n-hexane. Screening Value based on the TLV for n-hexane (110-54-3).
19550-03-9	2,3-Dimethyl-2-hexanol	n-Hexane	50	TLV	100	0.5	Very little information on 2,3-Dimethyl-2-hexanol; however, 2-hexanol, a potential metabolite, can be neurotoxic. 2-hexanol is also a metabolite of n-hexane. Screening Value based on the TLV for n-hexane (110-54-3).
623-37-0	3-Hexanol	2-Hexanol	60	TCLo	1000	0.06	No toxicity information located. TCLo - 270 mg/m3 (60 ppm) (RTECS). Screening value based on structural similarity to 2-hexanol (626-93-7), with additional uncertainty factor of 10 for use of a TCLo.
617-29-8	2-Methyl-3-hexanol	2-Hexanol	60	TCLo	1000	0.06	No toxicity information located. Screening value based on structural similarity to 2-hexanol, with additional uncertainty factor of 10 for use of a TCLo.
111-70-6	1-Heptanol	1-Octanol	50	WEEL	100	0.5	Screening Value based on structural similarity to 1-octanol (111-87-5).
543-49-7	2-Heptanol	1-Octanol	50	WEEL	100	0.5	Screening Value based on structural similarity to 1-octanol (111-87-5).
625-25-2	2-Methyl-2-heptanol	1-Octanol	50	WEEL	100	0.5	Screening Value based on structural similarity to 1-octanol (111-87-5).
19780-59-7	3-Ethyl-2-methyl-2-heptanol	1-Octanol	50	WEEL	100	0.5	Screening Value based on structural similarity to 1-octanol (111-87-5).
589-82-2	3-Heptanol	1-Octanol	50	WEEL	100	0.5	Screening Value based on structural similarity to 1-octanol (111-87-5).

Table A.3. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALKANOLS						
3913-02-8	2-Butyl-1-octanol	1-Octanol	50	WEEL	100	0.5	Rat oral LD50-13 gm/kg, very mild irritant. Toxicity may be less than for 1-octanol due to large size and steric hindrance. Screening Value based on structural similarities to 1-octanol (111-87-5).
123-96-6	2-Octanol	1-Octanol	50	WEEL	100	0.5	Screening Value based on structural similarity to 1-octanol (111-87-5).
628-44-4	2-Methyl-2-octanol	1-Octanol	50	WEEL	100	0.5	Although toxicity may be less than for 1-octanol due to large size and steric hindrance, Screening Value based on WEEL for 1-octanol (111-87-5).
19781-27-2	6-Ethyl-3-octanol	1-Octanol	50	WEEL	100	0.5	Although toxicity may be less than for 1-octanol due to large size and steric hindrance, Screening Value based on WEEL for 1-octanol (111-87-5).
57706-88-4	3,7-Dimethyl-3-octanol	1-Octanol	50	WEEL	100	0.5	Although toxicity may be less than for 1-octanol due to large size and steric hindrance, Screening Value based on WEEL for 1-octanol (111-87-5).
143-08-8	1-Nonanol	n.a.	n.a.	n.a.	100	0.07	Exposure of rats to concentrations as low as 7 ppm for 31 weeks caused neural toxicity and optic nerve damage (RTECS). Screening Value based on this information.
112-30-1	1-Decanol	n.a.	n.a.	n.a.	100	0.15	Rat - LD50 - ROUTE: Oral; DOSE: 4720 mg/kg (RTECS). One inhalation study in pregnant rats indicated the compound had little or no developmental or maternal toxicity at doses as high as 100 mg/m^3 (Nelson BK, et al., *J Am Col Toxic.* 1990, 9:93). Does not appear to be an irritant. Screening Value based on this information, 100 mg/m^3= 15.4 ppm as NOEL. A safety factor of 10 for screening should be conservative.
21078-65-9	2-Ethyl-1-decanol	1-Decanol	n.a.	n.a.	n.a.	0.015	No toxicity information located. Screening value based on similarity to 1-decanol (112-30-1). Add 100 SF for structural differences.
2425-77-6	2-Hexyl-1-decanol	n.a.	20	Danish EL	100	0.2	No toxicity information located, Danish recommended EL 200 mg/m3.

Table A.3. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALKANOLS						
1120-06-5	2-Decanol	1-Decanol	n.a.	n.a.	n.a.	0.015	No toxicity information located. Screening value based on structural similarity to 1-decanol (112-30-1). SF of 10 for surrogate use.
1565-81-7	3-Decanol	1-Decanol	n.a.	n.a.	n.a.	0.015	No toxicity information located. Screening value based on structural similarity to 1-decanol (112-30-1). SF of 10 for surrogate use.
5205-34-5	5-Decanol	1-Decanol	n.a.	n.a.	n.a.	0.015	No toxicity information located. Screening value based on structural similarity to 1-decanol (112-30-1). SF of 10 for surrogate use.
112-42-5	1-Undecanol	1-Decanol	n.a.	n.a.	n.a.	0.015	No toxicity information located. Screening value based on structural similarity to 1-decanol (112-30-1). SF of 10 for surrogate use.
1653-30-1	2-Undecanol	1-Decanol	n.a.	n.a.	n.a.	0.015	No toxicity information located. Screening value based on structural similarity to 1-decanol (112-30-1). SF of 10 for surrogate use.
4272-06-4	4-Undecanol	1-Decanol	n.a.	n.a.	n.a.	0.015	No toxicity information located. Screening value based on structural similarity to 1-decanol (112-30-1). SF of 10 for surrogate use.
112-53-8	1-Dodecanol	1-Decanol	n.a.	n.a.	n.a.	0.015	No toxicity information located. Screening value based on structural similarity to 1-decanol (112-30-1). SF of 10 for surrogate use.
10203-30-2	3-Dodecanol	1-Decanol	n.a.	n.a.	n.a.	0.015	No toxicity information located. Screening value based on structural similarity to 1-decanol (112-30-1). SF of 10 for surrogate use.
6836-38-0	6-Dodecanol	1-Decanol	n.a.	n.a.	n.a.	0.015	No toxicity information located. Screening value based on structural similarity to 1-decanol (112-30-1). SF of 10 for surrogate use.
1653-31-2	2-Tridecanol	1-Decanol	n.a.	n.a.	n.a.	0.015	No toxicity information located. Screening value based on structural similarity to 1-decanol (112-30-1). SF of 10 for surrogate use.

Table A.3. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALKANOLS						
112-72-1	1-Tetradecanol	1-Decanol	n.a.	n.a.	n.a.	0.015	Low toxicity, non-irritating. Rats exposed for up to 8 hr to saturated vapor had no lethality (Clayton, G. D. and F. E. Clayton, eds., *Patty's Industrial Hygiene and Toxicology*: Volume 2A, 2B, 2C; *Toxicology*. 3rd Ed. New York: John Wiley Sons, 1981-1982. p.4687). Screening Value based on this information and structural similarity to 1-decanol (112-30-1). SF of 10 for surrogate use.
629-76-5	1-Pentadecanol	1-Decanol	n.a.	n.a.	n.a.	0.015	No toxicity information located. Screening Value based on structural similarity to 1-decanol (112-30-1). SF of 10 for surrogate use.
36653-82-4	1-Hexadecanol	1-Decanol	n.a.	n.a.	n.a.	0.015	No toxicity information located. Screening Value based on structural similarity to 1-decanol (112-30-1). SF of 10 for surrogate use.
2490-48-4	2-Methyl-1-hexadecanol	1-Decanol	n.a.	n.a.	n.a.	0.0015	No toxicity information located. Screening Value based on structural similarity to 1-decanol (112-30-1). Added SF of 10 for structural differences
1454-85-9	1-Heptadecanol	1-Decanol	n.a.	n.a.	n.a.	0.015	No toxicity information located. Screening Value based on structural similarity to 1-decanol (112-30-1). SF of 10 for surrogate use.
41744-75-6	16-Methyl-1-heptadecanol	1-Decanol	n.a.	n.a.	n.a.	0.0015	No toxicity information located. Screening Value based on structural similarity to 1-decanol (112-30-1). Added SF of 10 for structural differences.
112-92-5	1-Octadecanol	1-Decanol	n.a.	n.a.	n.a.	0.015	No toxicity information located. Screening Value based on structural similarity to 1-decanol (112-30-1). SF of 10 for surrogate use.
1454-84-8	1-Nonadecanol	1-Decanol	n.a.	n.a.	n.a.	0.015	No toxicity information located, Screening Value based on structural similarity to 1-decanol (112-30-1).
	Incompletely Identified Alkanols						
53535-33-4	Heptanol	1-Ocanol	n.a.	n.a.	n.a.	0.5	No toxicity information located. Screening Value based on toxicity of 1-octanol .
28473-21-4	Nonanol	1-Nonanol	n.a.	n.a.	n.a.	0.07	No toxicity information located. Screening Value based on toxicity of 1-nonanol (143-08-8).

Table A.3. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	Incompletely Identified Alkanols						
26248-42-0	Tridecanol	1-Decanol	n.a.	n.a.	n.a.	0.0015	LD50 - ROUTE: Oral; DOSE: 4750 mg/kg (RTECS). Only other toxicity information available was in vitro mutagenicity data, all negative (HSDB). Screening Value based on structural similarity to 1-decanol (112-30-1). Added SF of 10 for structural differences
29354-98-1	Hexadecanol	1-Decanol	n.a.	n.a.	n.a.	0.0015	No toxicity information located. Screening Value based on structural similarity to 1-hexadecanol (36653-82-4). Added SF of 10 for structural dissimilarity.
	CYCLOALKANOLS						
96-41-3	Cyclopentanol	Cyclohexanol	50	TLV	100	0.5	Compound may cause dermatitis, pulmonary edema following inhalation exposure, and irritate mucous membranes (HSDB). Screening Value based on this information and similarity in structure to cyclohexanol (108-93-0).
2919-23-5	Cyclobutanol	Cyclohexanol	50	TLV	100	0.5	No toxicity information located. Screening Value based on structural similarity to cyclohexanol (108-93-0).
19550-46-0	1,3-Dimethylcyclopentanol	2-methylcyclohexanol	50	TLV	100	0.5	No toxicity information located. Screening Value based on structural similarity to 2-methylcyclohexanol (583-59-5).
591-23-1	3-Methylcyclohexanol	2-Methylcyclohexanol	50	Norway TWA	100	0.5	No toxicity information located. Screening Value based on structural similarity to 2-methylcyclohexanol (583-59-5).
4631-98-5	4-(1,1,3,3-Tetramethylbutyl) cyclohexanol	Cyclohexanol	50	TLV	100	0.5	No toxicity information located. Screening Value based on structural similarity to cyclohexanol (108-93-0).
470-65-5	4-Methyl-1-(1-methylethyl) cyclohexanol	Cyclohexanol	50	TLV	100	0.5	No toxicity information located. Screening Value based on structural similarity to cyclohexanol (108-93-0).
2407-94-5	1,1'-Dioxybiscyclohexanol	Cyclohexanol	50	TLV	100	0.5	No toxicity information located. Screening Value based on structural similarity to cyclohexanol (108-93-0).

Table A.3. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	CYCLOALKANOLS						
3761-94-2	1-Methylcycloheptanol	Cyclohexanol	50	TLV	100	0.5	No toxicity information located. Screening Value based on structural similarity to cyclohexanol (108-93-0).
13040-03-4	4,6,6-Trimethyl-(1a,2b,5a)-bicyclo[3.1.1]hept-3-en-2-ol	Cyclohexanol	50	TLV	100	0.5	No toxicity information located. Screening Value based on structural similarity to cyclohexanol (108-93-0).
30951-17-8	Decahydro-4a-methyl-8-methylene-2-(1-methylethyl)-1-naphthalenol	n.a.	n.a.	n.a.	n.a.	0.5	No information located for this or related compound. Screening Value set conservatively.
	ALKANDIOLS						
76-09-5	2,3-Dimethyl-2,3-butanediol	1,2-Propanediol	10	WEEL	100	0.1	Very little toxicity information located. Mouse, oral, LD50 9.0 ml/kg (HSDB). Screening Value based on structural similarity to 1,2-propanediol (57-55-6).
142-30-3	2,5-Dimethyl-3-hexyne-2,5-diol	1,2-Propanediol	10	WEEL	100	0.1	Very little toxicity information located. Mouse, intraperitoneal, LDlo >500 mg/kg (RTECS). Screening Value based on structural similarity to 1,2-propanediol (57-55-6).
19781-07-8	2,7-Dimethyl-2,7-octanediol	1-Octanol	50	WEEL	100	0.5	No information located. Screening Value based on structural similarity to 1-octanol (111-87-5).
5675-51-4	1,12-Dodecanediol	1-Decanol	n.a.	n.a.	n.a.	0.0015	No toxicity information located. Screening Value based on structural similarity to 1-decanol (112-30-1). Added SF of 10 for structural differences.
5057-99-8	trans-1,2-Cyclopentanediol	1,2-Propanediol	10	WEEL	100	0.1	No information located. Screening Value based on structural similarity to 1,2-propanediol (57-55-6).
	ALKENOLS, ALKENDIOLS, AND ALKYNEOLS						
4088-60-2	Z-2-Buten-1-ol	2-Buten-1-ol	n.a.	n.a.	n.a.	0.07	Surrogate: 2-Butene-1-ol (6117-91-5) racemic mixture; Rat-LCLo - ROUTE: Inhalation; DOSE: 2000 ppm/4H (RTECS). SF- 10 for surrogate, 10 for SF, 30 for LcLO.
627-27-0	3-Buten-1-ol	n.a.	n.a.	n.a.	n.a.	0.07	No toxicity information located. Screening Value based on structural similarity to 2-buten-1-ol (6117-91-5).

Table A.3. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALKENOLS, ALKENDIOLS, AND ALKYNEOLS						
598-32-3	3-Buten-2-ol	n.a.	n.a.	n.a.	n.a.	5	Screening value based on Human- TCLo - Inhalation - 50 ppm (RTECS).
39161-19-8	3-Penten-1-ol	2-Propen-1-ol	2	TWA	100	0.02	No toxicity information located. Screening Value based on structural similarity to 2-propen-1-ol (107-18-6).
1569-50-2	3-Penten-2-ol	2-Propen-1-ol	2	TWA	100	0.02	No toxicity information located. Screening Value based on structural similarity to 2-propen-1-ol (107-18-6).
922-65-6	1,4-Pentadien-3-ol	2-Propen-1-ol	2	TWA	100	0.02	No toxicity information located. Screening Value based on structural similarity to 2-propen-1-ol (107-18-6).
821-41-0	5-Hexen-1-ol	2-Propen-1-ol	2	TWA	100	0.02	No toxicity information located. Screening Value based on structural similarity to 2-propen-1-ol (107-18-6).
18521-07-8	Z-2-Methyl-3-octen-2-ol	1-Pentanol	100	WEEL	100	1	No toxicity information located. Screening Value based on structural similarity to 1-pentanol (71-41-0).
565-68-4	4-Methyl-1-pentyn-3-ol	1-Pentanol	100	WEEL	100	1	No toxicity information located. Screening Value based on structural similarity to 1-pentanol (71-41-0).
1482-15-1	3,4-Dimethyl-1-pentyn-3-ol	1-Pentanol	100	WEEL	100	1	No toxicity information located. Screening Value based on structural similarity to 1-pentanol (71-41-0).
74646-36-9	1-Dodecyn-4-ol	n.a.	n.a.	n.a.		1	No toxicity information located. Screening Value based high molecular weight relative to compounds like 5-Hexene-1-ol (821-41-0) and 1,4-pentadien-3-ol (922-65-6) where the Screening Value was set at 5 ppm.
51411-24-6	3,7,11-Trimethyl-6,10-dodecadien-1-ol	n.a.	n.a.	n.a.		1	No toxicity information located. Screening Value based high molecular weight relative to compounds like 5-Hexene-1-ol (821-41-0) and 1,4-pentadien-3-ol (922-65-6) where the Screening Value was set at 5 ppm.

Table A.3. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALKENOLS, ALKENDIOLS, AND ALKYNEOLS						
74646-37-0	1-Tridecyn-4-ol	n.a.	n.a.	n.a.		1	No toxicity information located. Screening Value based high molecular weight relative to compounds like 5-Hexene-1-ol (821-41-0) and 1,4-pentadien-3-ol (922-65-6) where the Screening Value was set at 5 ppm.
143-28-2	Z-9-Octadecen-1-ol	n.a.	n.a.	n.a.	n.a.	1	Oleyl alcohol; moderate to severe skin irritant in test species, mild in humans (RTECS). Screening Value based on this information.
	PHENOLS						
645-56-7	4-Propylphenol	2-sec-Butylphenol	5	TLV	100	0.05	Rat,TDLo - ROUTE: Oral; DOSE: 3640 mg/kg/26W intermittent, TOXIC EFFECTS: Liver - Hepatitis (hepatocellular necrosis), zonal; Endocrine - changes in adrenal weight (RTECS). Screening Value based on OEL for 2-sec-butylphenol (89-72-5), skin notation.
98-54-4	4-(1,1-Dimethylethyl)phenol	2-sec-Butylphenol	5	TLV	100	0.05	Screening Value based on OEL for 2-sec-butylphenol (89-72-5).
121-00-6	(1,1-Dimethylethyl)-4-methoxyphenol	2-sec-Butylphenol	5	TLV	100	0.05	Screening Value based on OEL for 2-sec-butylphenol (89-72-5).
25013-16-5	2-(1,1-Dimethylethyl)-4-methoxyphenol	2-sec-Butylphenol	5	TLV	100	0.05	Screening Value based on OEL for 2-sec-butylphenol (89-72-5).
608-25-3	2-Methyl-1,3-benzenediol	n.a.	n.a.	n.a.	n.a.	10	2-Methylresorcinol. Considered mild ocular irritant in rabbits and weak sensitizer in guinea pigs, but not humans (Anon. *J Am Coll Toxicol* 5(3):167-203, 1986). Screening Value based on this information.
136-77-6	4-Hexyl-1,3-benzenediol	n.a.	n.a.	n.a.	n.a.	0.2	Vesicant, irritating to respiratory tract and membranes, sensitizer in humans (HSDB). Screening Value based on this information.
	Incompletely Identified Phenols						
ARUP0-9	Di-t-butyl-ethylphenol	2-sec-Butylphenol	5	TLV	100	0.05	Screening Value based on OEL for 2-sec-butylphenol (89-72-5).
UPH000-01	Octylphenol	2-sec-Butylphenol	5	TLV	100	0.05	Screening Value based on OEL for 2-sec-butylphenol (89-72-5).

Table A.3. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	Incompletely Identified Phenols						
UPHUSI-01	Nonylphenol	2-sec-Butylphenol	5	TLV	100	0.05	Screening Value based on OEL for 2-sec-butylphenol (89-72-5).

Table A.4. Ethers

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ETHERS						
503-30-0	Trimethylene oxide	Isopropyl ether	250	TLV	100	2.5	Rat: LD50 - ROUTE: Subcutaneous; DOSE: 500 mg/kg (RTECS). Screening Value based on isopropyl ether (108-20-3).
110-71-4	1,2-Dimethoxyethane	n.a.	n.a.	n.a.	n.a.	100	Rat: Inhalation LCLo 63 g/m^3/6H; oral LDlo 1 gm/kg; Inhalation TCLo 16,000 mg/m^3/8D intermittent (RTECS). Screening Value based on this information.
628-28-4	1-Methoxybutane	2-Methyl-2-ethoxypropane	5	TLV	100	0.05	No reliable toxicity information located. Screening Value based on close structural relationship to 2-ethoxy-2-methylpropane (637-92-3).
61142-47-0	2-Methoxy-2-pentene	2-Methylpentane	500	TLV	1000	0.5	No toxicity information located. Screening Value based on structural similarity to 2-methylpentane (107-83-5). Structural similarity of this compound to surrogate is poor. Another surrogate, butylvinyl ether (111-34-2) caused 0/6 mortality in mice after exposure to 8,000 ppm for 4 hr (HSDB); however, no other data were found for this compound.
142-96-1	Dibutyl ether	n.a.	n.a.	n.a.	n.a.	1	Humans exposed to 100 ppm dibutyl ether estimated satisfactory for 8-hr exposures (Clayton, G. D. and F. E. Clayton [eds.]. *Patty's Industrial Hygiene and Toxicology*: Volume 2A, 2B, 2C; *Toxicology*. 3rd Ed. New York: John Wiley Sons, 1981-1982.2513). LC50 Rat inhalation 4,000 ppm/4 hr (HSDB). Use 100 ppm human exposure as NOEL, with SF of 100 for chronic exposures. Margin of exposure sufficiently high that this estimate is conservative.
628-80-8	1-Methoxypentane	2-Methyl-2-methoxybutane	20	TLV	100	0.2	No reliable toxicity information located. Screening Value based on close structural relationship to 2-methyl-2-methoxybutane (994-05-8).
56052-85-8	E-5-Pentyloxy-2-pentene	Dibutyl ether	n.a.	n.a.	n.a.	1	No toxicity information located. Screening Value based on structural similarity to dibutyl ether.
54658-01-4	3-Methoxyhexane	2-Methyl-2-ethoxypropane	5	TLV	100	0.05	No reliable toxicity information located. Screening Value based on close structural relationship to 2-ethoxy-2-methylpropane (637-92-3).

Table A.4. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ETHERS						
5756-43-4	1-Ethoxyhexane	2-Methyl-2-ethoxypropane	5	TLV	100	0.05	No reliable toxicity information located. Screening Value based on close structural relationship to 2-ethoxy-2-methylpropane (637-92-3).
42604-04-6	Methoxycycloheptane	2-Methyl-2-methoxybutane	20	TLV	100	0.2	No reliable toxicity information located. Screening Value based on structural relationship to tert-amyl methyl ether (994-05-8).
29887-79-4	trans-1,3-Dimethoxy cycloheptane	2-Methyl-2-methoxybutane	20	TLV	100	0.2	No reliable toxicity information located. Screening Value based on structural relationship to tert-amyl methyl ether (994-05-8).
2456-28-2	Didecyl ether	Dibutyl ether	n.a.	n.a.	n.a.	1	No toxicity information located. Screening Value based on structural similarity to dibutyl ether (142-96-1).
109-93-3	Divinyl ether	Vinyl methyl ether	n.a.	n.a.	n.a.	2	Little toxicity information located. Divinyl ether strongly mutagenic in Salmonella assay (Baden, et al., *Brit. J. Anaesthesia* 51:417-421) and induced sister-chromatid exchange in CHO cells (White et al., *Anesthesiology* 50(5):426-430, 1979). Used vinyl methyl ether (107-25-5) as surrogate. LC50 rat >64,000 ppm; TCLo rat 19,500 ppm-reproduction effects; TCLo rat 3,500 ppm 6H/DY/4W-various systemic effects (RTECS). Screening Value assigned on basis of this information
930-02-9	1-Ethenyloxyoctadecane	2-Ethoxy-2-methylpropane	n.a.	n.a.	n.a.	0.5	No toxicity information located. Screening Value based on structural similarity to 2-ethoxy-2-methylpropane (637-92-3). Structural similarity of this compound to surrogate is poor. Screening Value assigned may be excessively conservative. Another surrogate, butylvinyl ether (111-34-2) caused 0/6 mortality in mice after exposure to 8,000 ppm for 4 hr (HSDB); however, no other data were found for this compound.
20743-95-7	1-Butoxy-4-methoxybenzene	Diphenyl ether	1	Norway TWA	100	0.01	Screening Value based on structural similarity to diphenyl ether (101-84-8).
	Incompletely Identified Ethers						
UET005-01	C5-Ether	n.a.	n.a.	n.a.	n.a.	2	Screening Value based on consideration of structural possibilities.

Table A.5. Aldehydes

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALIPHATIC ALDEHYDES						
78-84-2	2-Methylpropanal	2-Methyl					
630-19-3	2,2-Dimethylpropanal	2-Methylpropanal	25	WEEL	100	0.25	Based on structural similarity to 2-methylpropanal (78-84-2).
96-17-3	2-Methylbutanal	Pentanal	50	TLV	100	0.5	Negative in mutagenicity assays (http://toxnet.nlm.nih.gov/cgi-bin/sis/search); rat LC50 14,000 ppm for 4 hr (http://www.matheson-trigas.com/msds/MAT27886.pdf). Screening Value based on structural similarity to pentanal (110-62-3).
590-86-3	3-Methylbutanal	Pentanal	50	TLV	100	0.5	Screening Value based on structural similarity to pentanal (110-62-3).
107-89-1	3-Hydroxybutanal	Crotonaldehyde	2	TLV	10	0.2	Screening Value based on structural similarity to Crotonaldehyde (123-73-9). SF reduced by 10 for lack of toxicity. LD50 in rats is 2180 mg/kg.
123-15-9	2-Methylpentanal	Pentanal	50	TLV	100	0.50	Screening Value based on structural similarity to pentanal (110-62-3) with additional safety factor of 3 to accommodate lower lethal concentration, 1500 ppm, 6 hr, rat (RTECS).
15877-57-3	3-Methylpentanal	Pentanal	50	TLV	300	0.17	No toxicity information located. Screening Value based on structural similarity to pentanal (110-62-3) with additional safety factor of 3 to accommodate lower lethal concentration, 1500 ppm, 6 hr, rat for 2-methylpentanal (RTECS).
66-25-1	Hexanal	Pentanal	50	TLV	10	5	Relatively non-toxic with respect to inhalation toxicity and lethality, but is an irritant (HSDB). Low toxicity reduces SF. Screening Value based on pentanal (110-62-3).
925-54-2	2-Methylhexanal	Hexanal	n.a.	n.a.	n.a.	1	No toxicity information located. Screening Value based on hexanal (66-25-1).
19269-28-4	3-Methylhexanal	Hexanal	n.a.	n.a.	n.a.	1	No toxicity information located. Screening Value based on hexanal (66-25-1).

Table A.5. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALIPHATIC ALDEHYDES						
123-05-7	2-Ethylhexanal	Pentanal	50	TLV	100	0.5	Relatively non-toxic with respect to inhalation toxicity and lethality, but is a slight irritant (HSDB). Screening Value based on pentanal (110-62-3).
111-71-7	Heptanal	Pentanal	50	TLV	100	0.5	RTECS indicates heptanal less toxic than pentanal based on LD50s and LC50s in rodents and skin irritation studies in rabbits. Screening Value based on pentanal (110-62-3).
124-13-0	Octanal	Pentanal	50	TLV	100	0.5	Very little toxicity information available although there is no indication of significant toxicity. Screening Value based on pentanal (110-62-3).
107-75-5	7-Hydroxy-3,7-dimethyloctanal	Pentanal	50	TLV	100	0.5	Very little toxicity information available although there is no indication of significant acute toxicity. The compound may be an irritant and sensitizer. Screening Value based on pentanal (110-62-3).
124-19-6	Nonanal	Pentanal	50	TLV	10	5	Very little toxicity information available although there is no indication of significant acute toxicity. Low toxicity reduces SF. The compound is an irritant in the Draize test. Screening Value based on pentanal (110-62-3).
112-31-2	Decanal	Pentanal	50	TLV	100	0.5	Very little toxicity information available although there is no indication of significant acute toxicity. The compound is an irritant in the Draize test. Screening Value based on pentanal (110-62-3).
112-44-7	Undecanal	Pentanal	50	TLV	100	0.5	Very little toxicity information available although there is no indication of significant acute toxicity. Screening Value based on pentanal (110-62-3).
110-41-8	2-Methylundecanal	Pentanal	50	TLV	100	0.5	Rat-LD50 - ROUTE: Oral; DOSE: >5 gm/kg (RTECS). Screening Value based on pentanal (110-62-3).
112-54-9	Dodecanal	Pentanal	50	TLV	100	0.5	Very little toxicity information available although there is virtually no acute toxicity. Screening Value based on pentanal (110-62-3).

Table A.5. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALIPHATIC ALDEHYDES						
10486-19-8	Tridecanal	Pentanal	50	TLV	100	0.5	Very little toxicity information available although there is no indication of significant acute toxicity. Screening Value based on pentanal (110-62-3).
629-80-1	Hexadecanal	Pentanal	50	TLV	100	0.5	Very little toxicity information available although there is no indication of significant acute toxicity. Screening Value based on pentanal (110-62-3).
	ALKENALS						
78-85-3	2-Methylprop-2-enal	Methacrylic acid	20	TLV	100	0.2	Screening value based on ACGIH-OEL for surrogate, methacrylic acid (79-41-4). Critical effect - irritation.
922-63-4	2-Methylenebutanal	Methacrylic acid	20	TLV	100	0.2	Screening value based on ACGIH-OEL for surrogate, methacrylic acid (79-41-4). Critical effect - irritation.
1115-11-3	2-Methylbut-2-enal	2-Butenal	0.3	PEL	100	0.003	No information located for this compound. As a member of the alpha-beta unsaturated aldehyde family it may be irritating and toxic. Screening Value based on these considerations and OSHA PEL for surrogate 2-butenal (crotonaldehyde; 4170-30-3). Surrogate is also classified as A3 by ACGIH, confirmed animal carcinogen.
5204-80-8	2-Ethylpent-4-enal	2,6-Dimethyl-5-heptenal	n.a.	n.a.	n.a.	5	For surrogate (106-72-9):Rat, oral, LD50 - >5mg/kg; Rabbit, skin, LD50 - >5mg/kg (*Food and Cosmetics Toxicology*, Vol. 13 (Suppl), Pg. 793, 1975). Screening Value based on data for surrogate.
645-62-5	2-Ethylhex-2-enal	2-Butenal	0.3	PEL	100	0.003	No information located for this compound. As a member of the alpha-beta unsaturated aldehyde family it may be irritating and toxic. Screening Value based on these considerations and OSHA PEL for surrogate 2-butenal (crotonaldehyde; 4170-30-3). Surrogate is also classified as A3 by ACGIH, confirmed animal carcinogen.

Table A.5. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALKENALS						
6728-26-3	E-Hex-2-enal	2-Butenal	0.3	PEL	100	0.003	No information located for this compound. As a member of the alpha-beta unsaturated aldehyde family it may be irritating and toxic. Screening Value based on these considerations and OSHA PEL for surrogate 2-butenal (crotonaldehyde; 4170-30-3). Surrogate is also classified as A3 by ACGIH, confirmed animal carcinogen.
6789-80-6	Z-Hex-3-enal	2,6-Dimethyl-5-heptenal	n.a.	n.a.	n.a.	5	For surrogate (106-72-9):Rat, oral, LD50 - >5mg/kg; Rabbit, skin, LD50 - >5mg/kg (*Food and Cosmetics Toxicology*, Vol. 13 (Suppl), Pg. 793, 1975). Screening value based on data for surrogate.
18829-55-5	E-Hept-2-enal	2-Butenal	0.3	PEL	100	0.003	No information located for this compound. As a member of the alpha-beta unsaturated aldehyde family it may be irritating and toxic. Screening Value based on these considerations and OSHA PEL for surrogate 2-butenal (crotonaldehyde; 4170-30-3). Surrogate is also classified as A3 by ACGIH, confirmed animal carcinogen.
6728-31-0	Z-Hept-4-enal	2,6-Dimethyl-5-heptenal	n.a.	n.a.	n.a.	5	For surrogate (106-72-9):Rat, oral, LD50 - >5mg/kg; Rabbit, skin, LD50 - >5mg/kg (*Food and Cosmetics Toxicology*, Vol. 13(Suppl), Pg. 793, 1975. Screening value based on data for surrogate.
106-72-9	2,6-Dimethylhept-5-enal	n.a.	n.a.	n.a.	n.a.	25	Rat, oral, LD50 - >5mg/kg; Rabbit, skin, LD50 - >5mg/kg (F*ood and Cosmetics Toxicology*, Vol. 13 (Suppl), Pg. 793, 1975).
2548-87-0	E-Oct-2-enal	2-Butenal	0.3	PEL	100	0.003	No information located for this compound. As a member of the alpha-beta unsaturated aldehyde family it may be irritating and toxic. Screening Value based on these considerations and OSHA PEL for surrogate 2-butenal (crotonaldehyde; 4170-30-3). Surrogate is also classified as A3 by ACGIH, confirmed animal carcinogen.

Table A.5. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALKENALS						
18829-56-6	E-Non-2-enal	2-Butenal	0.3	PEL	100	0.003	No information located for this compound. As a member of the alpha-beta unsaturated aldehyde family it may be irritating and toxic. Screening Value based on these considerations and OSHA PEL for surrogate 2-butenal (crotonaldehyde; 4170-30-3). Surrogate is also classified as A3 by ACGIH, confirmed animal carcinogen.
5910-87-2	E,E-Nona-2,4-dienal	2-Butenal	0.3	PEL	100	0.003	No information located for this compound. As a member of the alpha-beta unsaturated aldehyde family it may be irritating and toxic. Screening Value based on these considerations and OSHA PEL for surrogate 2-butenal (crotonaldehyde; 4170-30-3). Surrogate is also classified as A3 by ACGIH, confirmed animal carcinogen.
3913-81-3	E-Dec-2-enal	2-Butenal	0.3	PEL	100	0.003	No information located for this compound. As a member of the alpha-beta unsaturated aldehyde family it may be irritating and toxic. Screening Value based on these considerations and OSHA PEL for surrogate 2-butenal (crotonaldehyde; 4170-30-3). Surrogate is also classified as A3 by ACGIH, confirmed animal carcinogen.
97475-10-0	E,E-Dodeca-7,9-dienal	2,6-Dimethyl-5-heptenal	n.a.	n.a.	n.a.	5	For surrogate (106-72-9):Rat, oral, LD50 - >5mg/kg; Rabbit, skin, LD50 - >5mg/kg (F*ood and Cosmetics Toxicology*, Vol. 13(Suppl), Pg. 793, 1975). Screening value based on data for surrogate.
56554-96-2	Octadec-2-enal	2-Butenal	0.3	PEL	100	0.003	No information located for this compound. As a member of the alpha-beta unsaturated aldehyde family it may be irritating and toxic. Screening Value based on these considerations and OSHA PEL for surrogate 2-butenal (crotonaldehyde; 4170-30-3). Surrogate is also classified as A3 by ACGIH, confirmed animal carcinogen.

Table A.5. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALKENALS						
68820-35-9	E-Undec-4-enal	2,6-Dimethyl-5-heptenal	n.a.	n.a.	n.a.	5	For surrogate (106-72-9):Rat, oral, LD50 - >5mg/kg; Rabbit, skin, LD50 - >5mg/kg (*Food and Cosmetics Toxicology*, Vol. 13 (Suppl), Pg. 793, 1975). Screening value based on data for surrogate.
4826-62-4	Dodec-2-enal	2-Butenal	0.3	PEL	100	0.003	No information located for this compound. As a member of the alpha-beta unsaturated aldehyde family it may be irritating and toxic. Screening Value based on these considerations and OSHA PEL for surrogate 2-butenal (crotonaldehyde; 4170-30-3). Surrogate is also classified as A3 by ACGIH, confirmed animal carcinogen.
	Incompletely Identified Unsaturated Aldehydes						
UAD010-01	Decadienal	2-Butenal	0.3	PEL	100	0.003	No information located for this compound. As a member of the alpha-beta unsaturated aldehyde family it may be irritating and toxic. Screening Value based on these considerations and OSHA PEL for surrogate 2-butenal (crotonaldehyde; 4170-30-3). Surrogate is also classified as A3 by ACGIH, confirmed animal carcinogen.
	CYCLIC COMPOUNDS						
40702-26-9	1,3,4-Trimethylcyclohex-3-en-1-carboxaldehyde	2-Butenal	0.3	PEL	100	0.003	No information located for this compound. As a member of the alpha-beta unsaturated aldehyde family it may be irritating and toxic. Screening Value based on these considerations and OSHA PEL for surrogate 2-butenal (crotonaldehyde; 4170-30-3). Surrogate is also classified as A3 by ACGIH, confirmed animal carcinogen.
	AROMATIC ALDEHYDES						
123-08-0	4-Hydroxybenzaldehyde	Benzaldehyde	0.461	WEEL	100	0.0046	No toxicity data available. Screening Value based on benzaldehyde (100-52-7).

Table A.5. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	AROMATIC ALDEHYDES						
39515-51-0	3-Phenoxybenzaldehyde	Benzaldehyde	0.461	WEEL	200	0.0023	Rat: LC50 - 270 mg/m^3/4 hr; LD50 - 1222 mg/kg; Mouse LD50 1980 mg/kg (RTECS). Screening Value based on WEEL TLV for benzaldehyde. Although 3-phenoxybenzaldehyde appears to be less toxic than benzaldehyde via the oral route, it is more toxic via the inhalation route thus an additional safety factor of 2 was applied to the benzaldehyde TLV.

Table A.6. Ketones

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALIPHATIC KETONES						
75-97-8	3,3-Dimethyl-2-butanone	3-Methyl-2-butanone	200	TLV	100	2	RTECS LC50 5700 mg/m3 (1394 ppm); Screening Value based on structural similarity to 3-methyl-2-butanone (563-80-4) and 4-methyl-2-pentanone (108-10-1).
565-61-7	3-Methyl-2-pentanone	4-Methyl-2-pentanone	50	TLV	100	0.5	No toxicity data located; Screening Value based on structural similarity to 4-methyl-2-pentanone (108-10-1).
590-50-1	4,4-Dimethyl-2-pentanone	4-Methyl-2-pentanone	50	TLV	100	0.5	No toxicity data located; Screening Value based on structural similarity to 4-methyl-2-pentanone (108-10-1).
565-69-5	2-Methyl-3-pentanone	4-Methyl-2-pentanone	50	TLV	100	0.5	No toxicity data located; Screening Value based on structural similarity to 4-methyl-2-pentanone (108-10-1).
565-80-0	2,4-Dimethyl-3-pentanone	4-Methyl-2-pentanone	50	TLV	100	0.5	RTECS Rat LC50 from 2000 - 2765 ppm; HSDB no toxicity data; Screening Value based on structural similarity to 4-methyl-2-pentanone (108-10-1).
5857-36-3	2,2,4-Trimethyl-3-pentanone	4-Methyl-2-pentanone	50	TLV	100	0.5	No toxicity data located; Screening Value based on structural similarity to 4-methyl-2-pentanone (108-10-1).
105-42-0	4-Methyl-2-hexanone	2-Hexanone	5	TLV	100	0.05	No toxicity data located; Screening Value based on structural similarity to 2-hexanone (591-78-6).
14128-61-1	5-Methyl-5-phenyl-2-hexanone	Methyl isoamyl ketone	50	TLV	100	0.5	No toxicity data located. Screening Value based on structural similarity to methyl isoamyl ketone (110-12-3).
29006-00-6	6-Methoxy-3-hexanone	3-Pentanone	200	TLV	100	2	RTECS, Rat LCLo 4000 ppm/4 hr; structurally similar to 2-hexanone (591-78-6) but cannot form 2,5-hexanedione the neural toxic metabolite; also structurally similar to 3-pentanone (96-22-0) with TLV of 200 ppm.
UKE014-03	3-Cyclohexylidene-4-ethyl-2-hexanone	2-Hexanone	5	TLV	100	0.05	No toxicity data located; structurally similar compounds not identified; therefore, Screening Value based on 2-hexanone (591-78-6).
589-38-8	3-Hexanone	3-Pentanone	200	TLV	100	2	RTECS, Rat LCLo 4000 ppm/4 hr; structurally similar to 2-hexanone (591-78-6) but cannot form 2,5-hexanedione the neural toxic metabolite; also structurally similar to 3-pentanone (96-22-0) with TLV of 200 ppm.

Table A.6. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALIPHATIC KETONES						
1888-57-9	2,5-Dimethyl-3-hexanone	5-Methyl-2-hexanone	50	TLV	100	0.5	No toxicity data located; TLVs are available for three structurally related branched aliphatic ketones (i.e., 3-methyl-2-butanone (563-80-4), 2-methyl-4-pentanone (108-10-1), and 5-methyl-2-hexanone (110-12-3), with TLVs of 200, 50, and 50, respectively).
7379-12-6	2-Methyl-3-hexanone	Dipropyl ketone	50	TLV	100	0.5	Rat oral LD50 4 ml/kg. Similar to dipropyl ketone (123-19-3).
623-56-3	5-Methyl-3-hexanone	5-Methyl-2-hexanone	50	TLV	100	0.5	No toxicity data located. Screening Value set based on same rationale as for 2,5-dimethyl-3-hexanone (1888-57-9) above.
6137-12-8	4-Ethyl-3-hexanone	5-Methyl-2-hexanone	50	TLV	100	0.5	No toxicity data located. Screening Value set based on same rationale as for 2,5-dimethyl-3-hexanone (1888-57-9) above.
2371-19-9	3-Methyl-2-heptanone	2-Heptanone	50	TLV	100	0.5	No toxicity data located; Screening Value set based on structural similarity to 2-heptanone (110-43-0).
6137-06-0	4-Methyl-2-heptanone	2-Heptanone	50	TLV	100	0.5	No toxicity data located; Screening Value set based on structural similarity to 2-heptanone (110-43-0).
928-68-7	6-Methyl-2-heptanone	2-Heptanone	50	TLV	100	0.5	No toxicity data located; Screening Value set based on structural similarity to 2-heptanone (110-43-0).
19549-80-5	4,6-Dimethyl-2-heptanone	2-Heptanone	50	TLV	100	0.5	No toxicity data located; Screening Value set based on structural similarity to 2-heptanone (110-43-0).
624-42-0	6-Methyl-3-heptanone	5-Methyl-3-heptanone	25	TLV	100	0.25	TOMES 25 ppm produces strong odor, 50-100 ppm produces mild irritation to eyes, nose and throat and nausea and headache; rat oral LD50 3.5 g/kg - similar to 3-heptanone (106-35-4). Screening Value set based on structural similarity to 5-methyl-3-heptanone (541-85-5).
15726-15-5	3-Methyl-4-heptanone	4-Heptanone	50	TLV	100	0.5	TLV are available for three structurally related branched aliphatic ketones (i.e., 3-methyl-2-butanone (563-80-4), 2-methyl-4-pentanone (108-10-1), and 5-methyl-2-hexanone (110-12-3), with TLVs of 200, 50, and 50, respectively); Also structurally related to 4-heptanone (123-19-3), which has TLV 50 ppm.

Table A.6. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALIPHATIC KETONES						
111-13-7	2-Octanone	2-Heptanone	50	TLV	100	0.5	RTECS rat LC50 2132 ppm, Russian STEL 38 ppm. TLV based on structural similarity to 2-heptanone (110-43-0) and similar LC50 values and structural similarity to 2-heptanone (110-43-0).
589-63-9	4-Octanone	4-Heptanone	50	TLV	100	0.5	No toxicity data located. Screening Value set based on structural similarity to 4-heptanone (123-19-3).
20754-04-5	3-Methyl-4-octanone	5-Methyl-2-hexaone	50	TLV	100	0.5	No toxicity data located; TLVs are available for three structurally related branched aliphatic ketones (i.e., 3-methyl-2-butanone (563-80-4), 2-methyl-4-pentanone (108-10-1), and 5-methyl-2-hexanone (110-12-3), with TLVs of 200, 50, and 50, respectively).
821-55-6	2-Nonanone	2-Heptanone	50	TLV	100	0.5	RTECS Rat LC50 >687 ppm; TOXNET no useful data found. Screening Value based structural similarity to 2-heptanone (110-43-0).
925-78-0	3-Nonanone	3-Heptanone	50	TLV	100	0.5	No toxicity data located; food additive; Screening Value set based on similarity to 3-heptanone (106-35-4).
4485-09-0	4-Nonanone	4-Heptanone	50	TLV	100	0.5	No toxicity data located. Screening Value set based on structural similarity to 4-heptanone (123-19-3).
502-56-7	5-Nonanone	2-Hexanone	5	TLV	1000	0.005	RTECS Russian STEL 3.4 ppm, rat oral LD50 1g/kg; HSDB 5-nonanone metabolized by mice to hexane-2,5-dione the neuropathic metabolite of 2-hexanone and other gamma diketones, neurotoxicity observed in rats exposed orally at 233 mg/kg for 13 weeks. Add factor of 10 to account for neurotoxicity. Screening Value set based on similarity to 2-hexanone (591-78-6).
693-54-9	2-Decanone	2-Heptanone	50	TLV	100	0.5	RTECS Mouse oral LD50 7.9 g/kg; nephrotoxicity and α2u globin needs to be investigated. Screening Value based structural similarity to 2-heptanone (110-43-0).
33933-82-3	5,9-Dimethyl-2-decanone	4-Heptanone	50	TLV	100	0.5	No toxicity data located; Screening Value based on structural similarity to 4-heptanone (123-19-3); TLV are available for three structurally related branched aliphatic ketones (i.e., 3-methyl-2-butanone (563-80-4), 2-methyl-4-pentanone (108-10-1), and 5-methyl-2-hexanone (110-12-3), with TLVs of 200, 50, and 50, respectively).

Table A.6. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALIPHATIC KETONES						
928-80-3	3-Decanone	3-Heptanone	50	TLV	100	0.5	No toxicity data located; Screening Value based on structural similarity to 3-heptanone (106-35-4).
624-16-8	4-Decanone	4-Heptanone	50	TLV	100	0.5	No toxicity data located; Screening Value based on structural similarity to 4-heptanone (123-19-3).
820-29-1	5-Decanone	2-Heptanone	50	TLV	100	0.5	No toxicity data located; Screening Value based structural similarity to 2-heptanone (110-43-0).
112-12-9	2-Undecanone	2-Heptanone	50	TLV	100	0.5	RTECS mouse LC50 14,700 ppm. Screening Value based structural similarity to 2-heptanone (110-43-0).
1604-34-8	6,10-Dimethyl-2-undecanone	5-Methyl-2-hexaone	50	TLV	100	0.5	No toxicity data located; TLVs are available for three structurally related branched aliphatic ketones (i.e., 3-methyl-2-butanone (563-80-4), 2-methyl-4-pentanone (108-10-1), and 5-methyl-2-hexanone (110-12-3), with TLVs of 200, 50, and 50 respectively).
2216-87-7	3-Undecanone	3-Heptanone	50	TLV	100	0.5	No toxicity data located; Screening Value based on structural similarity to 3-heptanone (106-35-4).
14476-37-0	4-Undecanone	4-Heptanone	50	TLV	100	0.5	No toxicity data located; Screening Value based on structural similarity to 4-heptanone (123-19-3).
33083-83-9	5-Undecanone	2-Heptanone	50	TLV	100	0.5	No toxicity data located; Screening Value based structural similarity to 2-heptanone (110-43-0).
50639-02-6	2-Methyl-5-undecanone	2-Heptanone	50	TLV	100	0.5	No toxicity data located; Screening Value based on structural similarity to 2-heptanone (110-43-0).
6175-49-1	2-Dodecanone	2-Heptanone	50	TLV	100	0.5	No toxicity data located; Screening Value based structural similarity to 2-heptanone (110-43-0).
1534-27-6	3-Dodecanone	3-Heptanone	50	TLV	100	0.5	No toxicity data located; Screening Value based on structural similarity to 3-heptanone (106-35-4).
6137-26-4	4-Dodecanone	4-Heptanone	50	TLV	100	0.5	No toxicity data located; Screening Value based on structural similarity to 4-heptanone (123-19-3).
29366-35-6	11-Methyl-4-decanone	4-Heptanone	50	TLV	100	0.5	No toxicity data located; Screening Value based on structural similarity to 4-heptanone (123-19-3).
19780-10-0	5-Dodecanone	2-Heptanone	50	TLV	100	0.5	No toxicity data located; Screening Value based structural similarity to 2-heptanone (110-43-0).

Table A.6. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALIPHATIC KETONES						
6064-27-3	6-Dodecanone	4-Heptanone	50	TLV	100	0.5	TOMES no data by CAS number; TOXNET no data. No MSDS in SIRI. PubMed no toxicity information. Screening Value based on structural similarity to 4-heptanone (123-19-3).
593-08-8	2-Tridecanone	2-Heptanone	50	TLV	100	0.5	No toxicity data located; Screening Value based structural similarity to 2-heptanone (110-43-0).
1534-26-5	3-Tridecanone	3-Heptanone	50	TLV	100	0.5	No toxicity data located; Screening Value based on structural similarity to 3-heptanone (106-35-4).
26215-90-7	4-Tridecanone	4-Heptanone	50	TLV	100	0.5	No toxicity data located; Screening Value based on structural similarity to 4-heptanone (123-19-3).
30692-16-1	5-Tridecanone	2-Heptanone	50	TLV	100	0.5	No toxicity data located; Screening Value based structural similarity to 2-heptanone (110-43-0).
22026-12-6	6-Tridecanone	4-Heptanone	50	TLV	100	0.5	No toxicity data located; Screening Value based on structural similarity to 4-heptanone (123-19-3).
2345-27-9	2-Tetradecanone	2-Heptanone	50	TLV	100	0.5	No toxicity data located; Screening Value based structural similarity to 2-heptanone (110-43-0).
629-23-2	3-Tetradecanone	3-Heptanone	50	TLV	100	0.5	No toxicity data located; Screening Value based on structural similarity to 3-heptanone (106-35-4).
26496-20-8	4-Tetradecanone	4-Heptanone	50	TLV	100	0.5	No toxicity data located; Screening Value based on structural similarity to 4-heptanone (123-19-3).
502-69-2	6,10,14-Trimethyl-2-pentadecanone	2-Heptanone	50	TLV	100	0.5	No toxicity data located; Screening Value based on structural similarity to 2-heptanone (110-43-0).
2922-51-2	2-Heptadecanone	2-Heptanone	50	TLV	100	0.5	No toxicity data located; Screening Value based structural similarity to 2-heptanone (110-43-0).
	Incompletely Identified Ketones						
UKE006-01	C6-Alkanone	2-Hexanone	5	TLV	100	0.05	2-Hexanone is converted into 2,5-hexanedione, which is a strong neurotoxin. Screening Value is set based on 2-hexanone (591-78-6).
UKE007-02	C7-Alkanone	2-Heptanone	50	TLV	100	0.5	Screening Value based on 2-heptanone (110-43-0) with a 10X safety factor.
UKE008-01	C8-Alkanone	2-Heptanone	50	TLV	100	0.5	Screening Value based on 2-heptanone (110-43-0) with a 10X safety factor.

Table A.6. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	Incompletely Identified Ketones						
UKE009-03	C9-Alkanone	2-Heptanone	50	TLV	100	0.5	Screening Value based on 2-heptanone (110-43-0) with a 10X safety factor.
UKE010-01	C10-Alkanone	2-Heptanone	50	TLV	100	0.5	Screening Value based on 2-heptanone (110-43-0) with a 10X safety factor.
UKE011-02	C11-Alkanone	2-Heptanone	50	TLV	100	0.5	Screening Value based on 2-heptanone (110-43-0) with a 10X safety factor.
UKE012-02	C12-Alkanone	2-Heptanone	50	TLV	100	0.5	Screening Value based on 2-heptanone (110-43-0) with a 10X safety factor.
UKE013-02	C13-Alkanone	2-Heptanone	50	TLV	100	0.5	Screening Value based on 2-heptanone (110-43-0) with a 10X safety factor.
UKE014-01	C14-Alkanone	2-Heptanone	50	TLV	100	0.5	Screening Value based on 2-heptanone (110-43-0) with a 10X safety factor.
UKE006-03	4-Hydroxy-4-methylpentanone	4-Methyl-2-pentanone	50	TLV	1000	0.05	Screening Value based on structural similarity to 4-methyl-2- pentanone (108-10-1). A 10X safety factor was added to address the hydroxyl group.
	ALIPHATIC DIKETONES						
600-14-6	2,3-Pentadione	2-Pentanone and 3-Pentanone	200	TLV	1000	0.2	RTECS, rat oral LD50 3g/kg, LC50 not found. TOXNET included no information specific to 2,3-pentadione. SIRI MSDS with no useful toxicity data. Screening Value based on 2-petanone (107-87-9) and 3-pentanone (96-22-0) with additional safety factor of 10 due to structural differences.
110-13-4	2,5-Hexandione	2-Hexanone	5	TLV	1000	0.005	RTECS, rat LC50 2,000 ppm. TOXNET showed over 600 citations. No MSDS in SIRI. Based on comparison to 2-hexanone (591-78-6) with estimated LC50 of 20,000 ppm, an additional safety factor of 10 was applied due to structural differences.
1626-09-1	2,7-Octanedione	2-Hexanone	5	TLV	100	0.05	Limited toxicity information. Based on comparison to 2-hexanone (591-78-6)

Table A.6. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	CYCLOALKANONES						
UKE010-02	3-(2-Methyl-2-butyl) cyclopropanone	Cyclohexanone	20	TLV	300	0.067	No toxicity data located; Screening Value based on structural similarity to cyclohexanone (108-94-1). Additional safety factor of 3 due to potential reactivity of strained ring.
1191-95-3	Cyclobutanone	Cyclohexanone	20	TLV	300	0.067	No toxicity data located; Screening Value based on structural similarity to cyclohexanone (108-94-1). Additional safety factor of 3 due to potential reactivity of strained ring.
10374-14-8	2-Ethylcyclobutanone	Cyclohexanone	20	TLV	300	0.067	No toxicity data located; Screening Value based on structural similarity to cyclohexanone (108-94-1). Additional safety factor of 3 due to potential reactivity of strained ring.
1192-33-2	3,3-Dimethylcyclobutanone	Cyclohexanone	20	TLV	300	0.067	No toxicity data located; Screening Value based on structural similarity to cyclohexanone (108-94-1). Additional safety factor of 3 due to potential reactivity of strained ring.
28290-01-9	2,3,3-Trimethylcyclobutanone	Cyclohexanone	20	TLV	300	0.067	No toxicity data located; Screening Value based on structural similarity to cyclohexanone (108-94-1). Additional safety factor of 3 due to potential reactivity of strained ring.
1757-42-2	3-Methylcyclopentanone	Cyclohexanone	20	TLV	100	0.2	No toxicity data located; Screening Value based on structural similarity to cyclohexanone (108-94-1).
1121-33-1	2,4-Dimethylcyclopentanone	Cyclohexanone	20	TLV	100	0.2	No toxicity data located; Screening Value based on structural similarity to cyclohexanone (108-94-1).
19550-73-3	trans-3,4-Dimethyl cyclopentanone	Cyclohexanone	20	TLV	100	0.2	No toxicity data located; Screening Value based on structural similarity to cyclohexanone (108-94-1).
4573-09-5	2,2,5-Trimethyl cyclopentanone	Cyclohexanone	20	TLV	100	0.2	No toxicity data located; Screening Value based on structural similarity to cyclohexanone (108-94-1).
UKE010-02	3-(2-Methyl-2-butyl) cyclopentanone	Cyclohexanone	20	TLV	300	0.067	No toxicity data located; Screening Value based on structural similarity to cyclohexanone (108-94-1). Additional safety factor of 3 due to potential reactivity of strained ring.
69770-96-3	2-Methyl-4-(2-methylpropyl) cyclopentanone	Cyclohexanone	20	TLV	100	0.2	No toxicity data located; Screening Value based on structural similarity to cyclohexanone (108-94-1).

Table A.6. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	CYCLOALKANONES						
591-24-2	3-Methylcyclohexanone	Cyclohexanone	20	TLV	100	0.2	RTECS dog iv LD50 0.31 g/kg. Screening Value based on structural similarity to cyclohexanone (108-94-1).
16519-68-9	2,6-Dimethylcyclohexanone	Cyclohexanone	20	TLV	100	0.2	No toxicity data located; Screening Value based on structural similarity to cyclohexanone (108-94-1).
17429-02-6	4-Hydroxy-4-methyl cyclohexanone	Cyclohexanone	20	TLV	100	0.2	No toxicity data located; Screening Value based on structural similarity to cyclohexanone (108-94-1) and cyclohexanol (108-93-0; TLV = 50 ppm); also toluene (108-88-3; TLV = 50 ppm).
2408-37-9	2,2,6-Trimethylcyclohexanone	Cyclohexanone	20	TLV	100	0.2	No toxicity data located; Screening Value based on structural similarity to cyclohexanone (108-94-1).
873-94-9	3,3,5-Trimethylcyclohexanone	Cyclohexanone	20	TLV	100	0.2	RTECS rat LC50 2485 ppm. Screening Value based on structural similarity to cyclohexanone (108-94-1)
40649-36-3	4-Propylcyclohexanone	Cyclohexanone	20	TLV	100	0.2	No toxicity data located; Screening Value based on structural similarity to cyclohexanone (108-94-1).
15932-80-6	5-Methyl-2-(1-methylethylidene) cyclohexanone	Cyclohexanone	20	TLV	100	0.2	RTECS, Rat oral LD50 0.47 g/kg, rabbit skin LD50 3.09 g/kg. TOXNET common name pulegone, a component of peppermint. Appears to have toxicity to liver and other organs. Screening Value based on structural similarity to cyclohexanone (108-94-1).
89-82-7	5-Methyl-2-(1-methylethenyl) cyclohexanone	Cyclohexanone	20	TLV	100	0.2	RTECS, appears to be the same compound as CAS 15932-80-7. TOXNET common name pulegone, a component of peppermint. Appears to have toxicity to liver and other organs. Screening Value based on structural similarity to cyclohexanone (108-94-1).
637-88-7	1,4-Cyclohexanedione	Cyclohexanone	20	TLV	300	0.067	No toxicity data located; Screening Value based on structural similarity to cyclohexanone (108-94-1). Safety factor of 3 used due to potential reactivity of strained ring.
4176-04-9	4,7,7-Trimethylbicyclo-[4.1.0]heptan-3-one	Cyclohexanone	20	TLV	1000	0.02	No toxicity data located; limited structural similarity to cyclohexanone (108-94-1), thus an additional safety factor of 10X.

Table A.6. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALKENONES						
814-78-8	3-Methyl-3-buten-2-one	3-Buten-2-one	0.2	TLV Ceiling	100	0.002	RTECS, rat LCLo50 125 ppm; TOXNET little toxicity data, negative in Ames mutation test. Screening Value based on structural similarity to 3-buten-2-one (78-94-4) and comparison of LC50s.
763-93-9	3-Hexen-2-one	4-Methyl-3-penten-2-one (Mesityl oxide)	15	TLV	100	0.15	Alpha-beta unsaturated ketone. No toxicity data located; Screening Value based on structural similarity to 4-methyl-3-penten-2-one (141-79-7).
5166-53-0	5-Methyl-3-hexen-2-one	4-Methyl-3-penten-2-one (Mesityl oxide)	15	TLV	100	0.15	Alpha-beta unsaturated ketone. No toxicity data located; Screening Value based on structural similarity to 4-methyl-3-penten-2-one (141-79-7).
39899-08-6	3-Methyl-3-hepten-2-one	4-Methyl-3-penten-2-one (Mesityl oxide)	15	TLV	100	0.15	Alpha-beta unsaturated ketone. No toxicity data located; Screening Value based on structural similarity to 4-methyl-3-penten-2-one (141-79-7).
22319-25-1	4-Methyl-3-hepten-2-one	4-Methyl-3-penten-2-one (Mesityl oxide)	15	TLV	100	0.15	Alpha-beta unsaturated ketone. No toxicity data located; Screening Value based on structural similarity to 4-methyl-3-penten-2-one (141-79-7).
22319-29-5	5-Ethyl-2,4-dimethyl-4-hepten-3-one	4-Methyl-3-penten-2-one (Mesityl oxide)	15	TLV	100	0.15	Alpha-beta unsaturated ketone. No toxicity data located; Screening Value based on structural similarity to 4-methyl-3-penten-2-one (141-79-7).
110-93-0	6-Methyl-5-hepten-2-one	4-Methyl-3-penten-2-one (Mesityl oxide)	15	TLV	100	0.15	RTECS mammal (unspecified species) TCLo 228 ppm. TOXNET provided no useful data. IRIS MSDS rat oral LD50 3.5-4.25 g/kg. PubMed - no toxicity data. Screening Value based on structural similarity to 4-methyl-3-penten-2-one (141-79-7).
4312-99-6	1-Octen-3-one	4-Methyl-3-penten-2-one (Mesityl oxide)	15	TLV	100	0.15	Alpha-beta unsaturated ketone. No toxicity data located; Screening Value based on structural similarity to 4-methyl-3-penten-2-one (141-79-7).
1669-44-9	3-Octen-2-one	4-Methyl-3-penten-2-one (Mesityl oxide)	15	TLV	100	0.15	Alpha-beta unsaturated ketone. No toxicity data located. Screening Value based on structural similarity to 4-methyl-3-penten-2-one (141-79-7). Critical effect irritation, narcosis, liver, kidney.
14129-48-7	4-Octen-3-one	4-Methyl-3-penten-2-one (Mesityl oxide)	15	TLV	100	0.15	Alpha-beta unsaturated ketone. No toxicity data located; Screening Value based on structural similarity to 4-methyl-3-penten-2-one (141-79-7).

Table A.6. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALKENONES						
3664-60-6	7-Octen-2-one	4-Methyl-3-penten-2-one (Mesityl oxide)	15	TLV	100	0.15	No toxicity data located; Screening Value based on structural similarity to 4-methyl-3-penten-2-one (141-79-7).
51756-19-5	2-Methyl-1-nonen-3-one	4-Methyl-3-penten-2-one (Mesityl oxide)	15	TLV	100	0.15	Alpha-beta unsaturated ketone. No toxicity data located; Screening Value based on structural similarity to 4-methyl-3-penten-2-one (141-79-7).
32064-72-5	2-Nonen-4-one	4-Methyl-3-penten-2-one (Mesityl oxide)	15	TLV	100	0.15	Alpha-beta unsaturated ketone. No toxicity data located; Screening Value based on structural similarity to 4-methyl-3-penten-2-one (141-79-7).
3796-70-1	E-6,10-Dimethyl-5,9-undecadien-2-one	4-Methyl-3-penten-2-one (Mesityl oxide)	15	TLV	100	0.15	No toxicity data located; Screening Value based on structural similarity to 4-methyl-3-penten-2-one (141-79-7).
3879-26-3	Z-6,10-Dimethyl-5,9-undecadien-2-one	4-Methyl-3-penten-2-one (Mesityl oxide)	15	TLV	100	0.15	No toxicity data located; Screening Value based on structural similarity to 4-methyl-3-penten-2-one (141-79-7).
UKE015-01	4-Cyclohexylidene-3,3-diethyl-2-pentanone	4-Methyl-3-penten-2-one (Mesityl oxide)	15	TLV	100	0.15	No toxicity data located; Screening Value based on structural similarity to 4-methyl-3-penten-2-one (141-79-7).
42565-49-1	2,2,6,6-Tetramethyl-10-undecen-4-one	4-Methyl-3-penten-2-one (Mesityl oxide)	15	TLV	100	0.15	No toxicity data located; Screening Value based on structural similarity to 4-methyl-3-penten-2-one (141-79-7).
25564-22-1	2-Pentyl-2-cyclopenten-1-one	1,1,3-Trimethyl-3-cyclohexene-5-one (Isophorone)	5	TLV Ceiling	100	0.05	Rat: LD50 - ROUTE: oral; DOSE: 2200 mg/kg (RTECS). Screening Value based on structural similarity to 1,1,3-trimethyl-3-cyclohexene-5-one (78-59-1), an alpha-beta unsaturated ketone. ACGIH Ceiling 5 ppm. Critical effect: irritation, narcosis.
1121-05-7	2,3-Dimethyl-2-cyclopenten-1-one	1,1,3-Trimethyl-3-cyclohexene-5-one (Isophorone)	5	TLV Ceiling	100	0.05	Rat: LD50 - ROUTE: oral; DOSE: 2200 mg/kg (RTECS). Screening Value based on structural similarity to 1,1,3-trimethyl-3-cyclohexene-5-one (78-59-1), an alpha-beta unsaturated ketone. ACGIH Ceiling 5 ppm. Critical effect: irritation, narcosis.

Table A.6. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALKENONES						
83321-16-8	2,3,4-Trimethyl-3-cyclopenten-1-one	4-Methyl-3-penten-2-one (Mesityl oxide)	15	TLV	100	0.15	TOMES no data. TOXNET no data. No MSDS in SIRI. PubMed - no useful toxicity data. Screening Value based on structural similarity to 4-methyl-3-penten-2-one (141-79-7).
6711-26-8	2,5-Dimethyl-2-(1-methylethenyl) cyclohexanone	Cyclohexanone	20	TLV	1000	0.02	No toxicity data located; Screening Value based on structural similarity to cyclohexanone (108-94-1) with additional 10X safety factor for structural differences.
5715-25-3	4,5-Dimethyl-2-cyclohexen-1-one	Cyclohexanone	20	TLV	1000	0.02	No toxicity data located; Screening Value based on structural similarity to cyclohexanone (108-94-1) with additional 10X safety factor for alpha-beta unsaturated ketone.
17622-46-7	4-Ethyl-3,4-dimethyl-2-cyclohexen-1-one	Cyclohexanone	20	TLV	1000	0.02	No toxicity data located; Screening Value based on structural similarity to cyclohexanone (108-94-1) with additional 10X safety factor for alpha-beta unsaturated ketone.
35194-30-0	9-Decen-2-one	4-Methyl-3-penten-2-one (Mesityl oxide)	15	TLV	100	0.15	No toxicity data located; Screening Value based on structural similarity to 4-methyl-3-penten-2-one (141-79-7).
52588-78-0	6,6-Dimethyl-3,4-undecadien-2,10-dione	4-Methyl-3-penten-2-one (Mesityl oxide)	15	TLV	1000	0.015	No toxicity data located; Screening Value based on structural similarity to 4-methyl-3-penten-2-one (141-79-7) with additional 10X safety factor for alpha-beta unsaturated ketone.
	Incompletely Identified Alkenones						
UKE006-02	C6-Alkenone	4-Methyl-3-penten-2-one (Mesityl oxide)	15	TLV	100	0.15	Screening Value based structural similarity to 4-methyl-3-penten-2-one (141-79-7).
UKE009-02	C9-Alkenone	4-Methyl-3-penten-2-one (Mesityl oxide)	15	TLV	100	0.15	Screening Value based structural similarity to 4-methyl-3-penten-2-one (141-79-7).
	AROMATIC KETONES AND QUINONES						
26465-81-6	2,3-Dihydro-3,3-dimethyl-1H-inden-1-one	Indene	10	TLV	1000	0.01	No toxicity data located; Screening Value based on structural similarity to indene (95-13-6) with ACGIH TLV of 10 ppm - an additional 10X safety factor is recommended for structural differences.

Table A.6. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	AROMATIC KETONES AND QUINONES						
2040-07-5	1-(2,4,5-Trimethylphenyl) ethanone	Acetophenone	10	TLV	100	0.1	No toxicity data located; Screening Value based on structural similarity to acetophenone (98-86-2).
585-74-0	1-(3-Methylphenyl)ethanone	Acetophenone	10	TLV	100	0.1	No toxicity data located; Screening Value based on structural similarity to acetophenone (98-86-2).
705-15-7	1-(2-Hydroxy-5-methoxyphenyl)ethanone	Acetophenone	10	TLV	100	0.1	No toxicity data located; Screening Value based on structural similarity to acetophenone (98-86-2).
1506-02-1	1-(5,6,7,8-Tetrahydro-3,5,5,6,8,8-hexamethyl-2-naphthenyl)ethanone	Acetophenone	10	TLV	100	0.1	RTECS no acute data available. 2-week oral study gave TDLo of 0.091g/kg/2 weeks (liver weight increase) and 90-day oral study gave TDLo of 4.5 g/kg/90 days (increased liver weight and changes in erythrocyte count and pigmentation). Not mutagenic in microbial assay and not genotoxic in human cell micronucleus test. Screening Value based on structural similarity to acetophenone (98-86-2).
1009-61-6	bis-1,1'-(1,4-Phenylene) ethanone	Acetophenone	10	TLV	100	0.1	No toxicity data located; Screening Value based on structural similarity to acetophenone (98-86-2).
93-55-0	1-Phenyl-1-propanone	Acetophenone	10	TLV	100	0.1	RTECS rat oral LD50 4.49 ml/kg. Screening Value based on structural similarity to acetophenone (98-86-2).
486-25-9	9H-Fluoren-9-one	Acetophenone	10	TLV	1000	0.01	RTECS mouse ip LD50 >2g/kg. Screening Value based on structural similarity to acetophenone (98-86-2) with additional 10X safety factor for structural differences.
719-22-2	2,6-bis(1,1-Dimethylethyl)-2,5-cyclohexdiene-1,4-dione	Acetophenone	10	TLV	1000	0.01	RTECS mouse ip LD50 2.27 g/kg. HSDB benzoquinones form radicals. TOXNET, chronic neurotoxic effects including vision disturbances. Screening Value based on structural similarity to acetophenone (98-86-2) with additional safety factor of 10X.

Table A.7. Organic Acids

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALKANOIC ACIDS						
79-31-2	2-Methylpropionic acid	Propanoic acid	10	TLV	10	1	Rat:LD50 - ROUTE: oral; DOSE: 280 µL/kg (RTECS); Screening Value based on TLV for propanoic acid (79-09-4).
107-92-6	Butanoic acid	Propanoic acid	10	TLV	10	1	RTECS rat and mouse LC50 >139ppm. TOXNET considerable toxicity data. It is a product of fatty acid metabolism and a food additive. Mild irritant. Screening Value based on structural similarity to propanoic acid (79-09-4) and acetic acid (64-19-7; TLV = 10 ppm).
142-62-1	Hexanoic acid	Propanoic acid	10	TLV	10	1	RTECS rat LC 50 of 4100 mg/m3/2 hours (865 ppm). Screening Value based on structural similarity to propanoic acid (79-09-4) and acetic acid (64-19-7; TLV = 10 ppm).
334-48-5	Decanoic acid	n.a.	n.a.	n.a.	n.a.	1	HSDB: No irritation to human skin at 1% petroleum solution; mouse LD50, i.v., 130 mg/kg. Readily metabolized in two carbon units. Natural product.
143-07-7	Dodecanoic acid	Decanoic acid	n.a.	n.a.	n.a.	1	Decanoic acid (334-48-5) HSDB data: no irritation to human skin at 1% petroleum solution; mouse LD50, i.v., 130 mg/kg. Readily metabolized in two carbon units. Natural product.
544-63-8	Tetradecanoic acid	Decanoic acid	n.a.	n.a.	n.a.	1	Decanoic acid (334-48-5) HSDB data: no irritation to human skin at 1% petroleum solution; mouse LD50, i.v., 130 mg/kg. Readily metabolized in two carbon units. Natural product.
5746-58-7	12-Methyltetradecanoic acid	Decanoic acid	n.a.	n.a.	n.a.	1	Decanoic acid (334-48-5) HSDB data: no irritation to human skin at 1% petroleum solution; mouse LD50, i.v., 130 mg/kg. Readily metabolized in two carbon units. Natural product.
1002-84-2	Pentadecanoic acid	Decanoic acid	n.a.	n.a.	n.a.	1	Decanoic acid (334-48-5) HSDB data: no irritation to human skin at 1% petroleum solution; mouse LD50, i.v., 130 mg/kg. Readily metabolized in two carbon units. Natural product.
57-10-3	Hexadecanoic acid	Decanoic acid	n.a.	n.a.	n.a.	1	Decanoic acid (334-48-5) HSDB data: no irritation to human skin at 1% petroleum solution; mouse LD50, i.v., 130 mg/kg. Readily metabolized in two carbon units. Natural product.
57-11-4	Octadecanoic acid	n.a.	n.a.	n.a.	n.a.	1	Stearic acid. Regulated as particulate at 10 mg/m^3.
1759-53-1	Cyclopropanecarboxylic acid	Propanoic acid	10	TLV	100	0.1	Mouse: LD50 - ROUTE: Intravenous; DOSE: 180 mg/kg (RTECS); Screening Value based on structural similarity to propanoic acid (79-09-4); critical effect: irritation.

Table A.7. (contdd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALKANOIC ACIDS						
1123-28-0	1-Hydroxycyclohexane carboxylic acid	n.a.	n.a.	n.a.	n.a.	0.3	No toxicity information located. Screening Value based on toxicity of similar compounds, 1-methylhydroxycyclohexanecarboxylic acid (11123-25-7) mouse iv LD50 840 mg/kg and cyclohexancarboxylic acid (98-89-5) rat oral LD50 3265 mg/kg (RTECS). Estimated screening value based on this information.
27392-16-1	trans-2-(1,1-Dimethylethyl)-cyclohexanecarboxylic acid	2-Ethylhexanoic acid	0.66	TLV	1000	0.00066	No toxicity information located. Screening Value based on structural similarity to acetic acid (64-19-7), propanoic acid (79-09-4), and 2-ethylhexanoic acid (149-57-5; TLV = 5 mg/m3) (chain branching); therefore 10X safety factor added.
	Incompletely Identified Alkanoic Acids						
UCA014-01	C14-Alkanoic acid	Decanoic acid	n.a.	n.a.	n.a.	1	Decanoic acid (334-48-5) HSDB data: no irritation to human skin at 1% petroleum solution; mouse LD50, i.v., 130 mg/kg. Readily metabolized in two carbon units. Natural product.
UCA016-01	C16-Alkanoic acid	Decanoic acid	n.a.	n.a.	n.a.	1	Decanoic acid (334-48-5) HSDB data: no irritation to human skin at 1% petroleum solution; mouse LD50, i.v., 130 mg/kg. Readily metabolized in two carbon units. Natural product.
	ALKENOIC ACIDS						
17351-34-7	Pentadec-14-enoic acid	Decanoic acid	n.a.	n.a.	n.a.	1	Decanoic acid (334-48-5) HSDB data: no irritation to human skin at 1% petroleum solution; mouse LD50, i.v., 130 mg/kg. Readily metabolized in two carbon units. Natural product.
2091-29-4	Hexadec-9-enoic acid	Decanoic acid	n.a.	n.a.	n.a.	1	Decanoic acid (334-48-5) HSDB data: no irritation to human skin at 1% petroleum solution; mouse LD50, i.v., 130 mg/kg. Readily metabolized in two carbon units. Natural product.
112-80-1	Z-Octadec-9-enoic acid	Decanoic acid	n.a.	n.a.	n.a.	1	Decanoic acid (334-48-5) HSDB data: no irritation to human skin at 1% petroleum solution; mouse LD50, i.v., 130 mg/kg. Readily metabolized in two carbon units. Natural product.
	OTHER ACIDS						
79-14-1	Glycolic acid	n.a.	n.a.	n.a.	n.a.	1.2	Rat-LC50 - ROUTE: Inhalation; 3.6 mg/L (1157 ppm). NOEL for developmental effects 150 mg/kg/day. Oral rat LD50 1938 mg/kg. This Screening Value is based on the inhalation LC50.

Table A.7. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	OTHER ACIDS						
298-12-4	Glyoxylic acid	n.a.	n.a.	n.a.	n.a.	12	Rat-LDLo - ROUTE: Oral; DOSE: 3 gm/kg (RTECS). Screening value based on structural similarity to glycolic acid, but LD50/LDLo indicates much less toxic potential.
56-40-6	Glycine	n.a.	n.a.	n.a.	n.a.	100	Glycine has not been shown to be overtly toxic or irritating in reasonable quantities, i.e., less than several grams (HSDB 2002). Screening Value based on HSDB comment.

Table A.8. Esters

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALKANE ESTERS						
110-74-7	Propyl formate	Ethyl formate	100	TLV	100	1	RTECS rat oral LD50 3980 mg/kg, mouse oral LD50 3400 mg/kg. Screening Value based on structural similarity to ethyl formate (109-97-4).
542-55-2	2-Methylpropyl formate	Methyl formate	100	TLV	100	1	Rabbit oral LD50 3.064 g/kg (RTECS). Screening Value based on structural similarity to methyl formate (107-31-3).
1838-59-1	2-Propenyl formate	Methyl formate	100	TLV	100	1	Rat LC50 980 mg/m3 (279 ppm) (RTECS). Also known as allyl formate - induces severe hepatic injury. Screening Value based on structural similarity to methyl formate (107-31-3) and information on liver toxicity.
592-84-7	Butyl formate	Methyl formate	100	TLV	100	1	Human inhalation TCLo 10,418 ppm. Rabbit oral LD50 2.656 g/kg. (RTECS) Screening Value based on structural similarity to methyl formate (107-31-3).
591-87-7	2-Propenyl acetate	n.a.	50	UK TWA	10	5	Rat LC50 1000 ppm. Rat oral LD50 0.13 g/kg. It is absorbed through intact skin. (RTECS) Strong irritant and hepatotoxin.
35468-97-4	1-Hepten-1-yl acetate	Butyl acetate	150	TLV	100	1.5	No toxicity information located. Screening Value based on structural similarity to butyl acetate (123-86-4).
629-70-9	1-Hexadecyl acetate	Butyl acetate	150	TLV	100	1.5	Rat oral LD50 >5g/kg (RTECS). Screening Value based on structural similarity to butyl acetate (123-86-4).
OHUES0-01	1-Heptadecanyl acetate	Butyl acetate	150	TLV	100	1.5	No toxicity information located. Screening Value based on structural similarity to butyl acetate (123-86-4).
6295-06-3	Butyl glyoxalate	Butyl acetate	150	TLV	100	1.5	No toxicity information located. Screening Value based on structural similarity to butyl acetate (123-86-4).
1932-92-9	2-Propyn-1-yl propanioate	Butyl acetate	150	TLV	100	1.5	No toxicity information located. Screening Value based on structural similarity to butyl acetate (123-86-4).
590-01-2	Butyl propionate	Butyl acetate	150	TLV	100	1.5	RTECS Rat oral LD50 5 g/kg. Rabbit eye - severe irritation. Screening Value based on structural similarity to butyl acetate (123-86-4).
142-60-9	Octyl propionate	Butyl acetate	150	TLV	100	1.5	No toxicity information located. Screening Value based on structural similarity to butyl acetate (123-86-4).
74381-40-1	1-(1,1-Dimethylethyl)-2-methyl-1,3-propanediyl 2-methylpropanoate	Propanoic acid	10	TLV	100	0.1	No toxicological information. Compound has potential to cleave into propanoic acid (57-57-8). ACGIH TLV for propanoic acid, 10 ppm. Critical effect: irritation.

Table A.8. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALKANE ESTERS						
97-87-0	Butyl 2-methylpropionate	Butyl acetate	150	TLV	100	1.5	RTECS Rat oral LD50 >5g/kg. Screening Value based on structural similarity to butyl acetate (123-86-4) with additional 10X safety factor.
74367-34-3	3-Hydroxy-2,4,4-trimethylpentyl-2-methylpropanoate	Butyl acetate	150	TLV	1000	0.15	No toxicity information located. Screening Value based on structural similarity to butyl acetate (123-86-4) with additional 100X safety factor for hydroxyl- and branched chain functional groups.
105-66-8	Propyl butanoate	n.a.	n.a.	n.a.	n.a.	15	Little toxicity information located. Rat oral LD50 15000 mg/kg. Screening Value based on high oral LD50.
819-97-6	1-Methylpropyl butanoate	Butyl acetate	150	TLV	100	1.5	No toxicity information located. Screening Value based on structural similarity to butyl acetate (123-86-4) with additional 10X safety factor.
109-21-7	Butyl butanoate	Butyl acetate	150	TLV	100	1.5	TOMES RTECS Rabbit oral LD50 9.520 g/kg. Moderate skin irritation in rabbit. TOXNET provided no useful data. Screening Value based on structural similarity to butyl acetate (123-86-4) with additional 10X safety factor.
53398-83-7	E-2-Hexenyl butanoate	Butyl acetate	150	TLV	100	1.5	No toxicity information located. Screening Value based on structural similarity to butyl acetate (123-86-4) with additional 10X safety factor for double bond.
2639-63-6	Hexyl butanoate	Butyl acetate	150	TLV	100	1.5	RTECS Rat oral LD50 >5g/kg. Mild skin irritant in rabbit. Screening Value based on structural similarity to butyl acetate (123-86-4) with additional 10X safety factor.
123-25-1	Diethyl butanedioate	Butyl acetate	150	TLV	100	1.5	Rat oral LD50 8.530 g/kg. Mild skin and eye irritant. (RTECS) Screening Value based on structural similarity to butyl acetate (123-86-4) with additional 10X safety factor.
20474-93-5	2-Propenyl 2-butenoate	Butyl acetate	150	TLV	1000	0.15	No toxicity information located. Screening Value based on structural similarity to butyl acetate (123-86-4) with additional 10X safety factor for double bond.
1117-59-5	Hexyl pentanoate	Butyl acetate	150	TLV	100	1.5	No toxicity information located. Screening Value based on structural similarity to butyl acetate (123-86-4) with additional 10X safety factor.
3682-42-6	Methyl 2-oxo-3-methylpentanoate	Butyl acetate	150	TLV	100	1.5	No toxicity information located. Screening Value based on structural similarity to butyl acetate (123-86-4) with additional 10X safety factor for oxo-group.

Table A.8. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALKANE ESTERS						
68443-63-0	Butyl 2-ethylhexanoate	Butyl acetate	150	TLV	1000	0.15	No toxicity information located. Screening Value based on structural similarity to butyl acetate (123-86-4) with additional 100X safety factor for carcinogenic response for Dioctyl hexandioate.
38447-22-2	bis(1-Methylpropyl) hexanedioate	Butyl acetate	150	TLV	1000	0.15	No toxicity information located. Screening Value based on structural similarity to butyl acetate (123-86-4) with additional 100X safety factor for carcinogenic response for dioctyl hexandioate, a related compound.
123-79-5	Dioctyl hexandioate	Butyl acetate	150	TLV	1000	0.15	RTECS Rat oral LD50 7.392 g/kg. Reproduction effects at high doses. Tumorigenic in mice (liver) by RTECS criteria. Screening Value based on structural similarity to butyl acetate (123-86-4) with additional 100X safety factor for carcinogenic response in mice.
4337-65-9	2-Ethylhexyl hexandioate	Butyl acetate	150	TLV	1000	0.15	No toxicity information located. Screening Value based on structural similarity to butyl acetate (123-86-4) with additional 100X safety factor for carcinogenic response in mice.
103-23-1	bis(2-Ethylhexyl) hexandioate	Butyl acetate	150	TLV	1000	0.15	Rat oral LD50 7.392 g/kg. Feeding study of mice resulted in liver tumors. Also reproductive effects at high doses (around 15 g/kg) (RTECS). Screening Value based on structural similarity to butyl acetate (123-86-4) with additional 100X safety factor for carcinogenic response for dioctyl hexandioate.
54845-28-2	(E,E)-2-Hexenyl 2-hexenoate	Butyl acetate	150	TLV	1000	0.15	No toxicity information located. Screening Value based on structural similarity to butyl acetate (123-86-4) with additional 100X safety factor for carcinogenic response for dioctyl hexandioate.
69687-91-8	4-Methylphenyl 2-hexenoate	Butyl acetate	150	TLV	1000	0.15	No toxicity information located. Screening Value based on structural similarity to butyl acetate (123-86-4) with additional 100X safety factor for carcinogenic response for dioctyl hexandioate.
5454-28-4	Butyl heptanoate	Butyl acetate	150	TLV	1000	0.15	No toxicity information located. Screening Value based on structural similarity to butyl acetate (123-86-4) with additional 100X safety factor for carcinogenic response for dioctyl hexandioate.

Table A.8. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALKANE ESTERS						
UES013-01	1-Ethylpropyl octanoate	Butyl octadecanoate	0.35	Sweden TWA	100	0.0035	No toxicity information located. Screening Value based on structural similarity to butyl octadecanoate (butyl stearate; 123-95-5).
110-27-0	1-Methylethyl tetradecanoate	Butyl octadecanoate	0.35	Sweden TWA	100	0.0035	RTECS rat oral LD50 >16 g/kg. Irritant to rabbit skin. Screening Value based on structural similarity to butyl octadecanoate (123-95-5).
110-36-1	Butyl tetradecanoate	Butyl octadecanoate	0.35	Sweden TWA	100	0.0035	RTECS rat oral LD50 >8g/kg. Irritant to rabbit skin. Considered safe for cosmetic use (Elder, RL. *J. Amer. College Tox.* 9, 247-258, 1990). Screening Value based on structural similarity to butyl octadecanoate (123-95-5).
35996-97-5	Butyl pentadecanoate	Butyl octadecanoate	0.35	Sweden TWA	100	0.0035	No toxicity information located. Screening Value based on structural similarity to butyl octadecanoate (123-95-5).
142-91-6	1-Methylethyl hexadecanoate	Butyl octadecanoate	0.35	Sweden TWA	100	0.0035	RTECS rat oral LD50 >5 g/kg. Moderate irritant to rabbit skin. Screening Value based on structural similarity to butyl octadecanoate (123-95-5).
542-44-9	2,3-Dihydroxypropyl hexadecanoate	Butyl octadecanoate	0.35	Sweden TWA	100	0.0035	No toxicity information located. Screening Value based on structural similarity to butyl octadecanoate (123-95-5).
111-06-8	Butyl hexadecanoate	Butyl octadecanoate	0.35	Sweden TWA	100	0.0035	No toxicity information located. Screening Value based on structural similarity to butyl octadecanoate (123-95-5).
123-95-5	Butyl octadecanoate	Butyl octadecanoate	0.35	Sweden TWA	100	0.0035	Screening Value based on Swedish TLV. RTECS rat oral LD50 32 g/kg. Rabbit moderate skin irritant. Reproductive effects.
1937-62-8	Methyl E-9-octadecenoate	Butyl octadecanoate	0.35	Sweden TWA	100	0.0035	No toxicity information located. Screening Value based on structural similarity to butyl octadecanoate (123-95-5).
20698-91-3	Methyl α-hydroxybenzeneacetate	Butyl octadecanoate	0.35	Sweden TWA	100	0.0035	No toxicity information located. Screening Value based on structural similarity to butyl octadecanoate (123-95-5) and to di-(2-ethylhexyl) phthalate (117-81-7).
774-40-3	Ethyl α-hydroxybenzeneacetate	Butyl octadecanoate	0.35	Sweden TWA	100	0.0035	RTECS mouse oral LD50 3.75 g/kg. Severe eye irritant in rabbit. Screening Value based on structural similarity to butyl octadecanoate (123-95-5) and to di-(2-ethylhexyl) phthalate (117-81-7).

Table A.8. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	Incompletely Identified Aliphatic Esters						
UES010-01	C6 Ester of butanoic acid	Butyl acetate	150	TLV	1000	0.15	Hexyl butanoate is listed above with Screening Value of 15 ppm. Screening Value based on structural similarity to butyl acetate with a 1000X safety factor due to lack of toxicity data.
	BENZENE ESTERS						
84-64-0	Butyl cyclohexyl phthalate	Diethyl phthalate	0.55	TLV	10	0.055	HSDB phthalates have low acute toxicity, may be irritants to skin, eye and respiratory tract. Reduced SF due to low toxicity. Screening Value based on structural similarity to diethyl phthalate (84-66-2).
17851-53-5	Butyl 2-methylpropyl phthalate	Diethyl phthalate	0.55	TLV	100	0.0055	No toxicity information located. Screening Value based on structural similarity to diethyl phthalate (84-66-2).
85-69-8	Butyl 2-ethylhexyl phthalate	Diethyl phthalate	0.55	TLV	100	0.0055	No toxicity information located. Screening Value based on structural similarity to diethyl phthalate (84-66-2).
26537-19-9	Methyl 4-(1,1-dimethylethyl)benzoate	Diethyl phthalate	0.55	TLV	1000	0.00055	No toxicity information located. Screening Value based on structural similarity to diethyl phthalate (84-66-2). With additional factor of 10 for structural differences
	PHOSPHATE ESTERS						
78-46-6	Dibutyl butylphosphonate	Tributyl phosphate	0.2	TLV	100	0.002	RTECS mouse LDLo ip 0.125g/kg. Mouse LD50 iv 0.056 g/kg. Insect (tick) repellant. Screening Value based on structural similarity to tributyl phosphate (126-73-8).

Table A.9. Nitriles

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALKANE NITRILES						
630-18-2	2,2-Dimethylpropanenitrile	2-Methylpropanenitrile	8	REL	100	0.08	No toxicity information located. Based on structural similarity to 2-methyl propanenitrile (78-82-0).
18936-17-9	2-Methylbutanenitrile	2-Methylpropanenitrile	8	REL	100	0.08	No toxicity information located. Based on structural similarity to 2-methyl propanenitrile (78-82-0).
1647-11-6	2-Methylene butanenitrile	Acrylonitrile	2	TLV	100	0.02	Based on structural similarity to acrylonitrile (107-13-1).
110-59-8	Pentanenitrile	Butanenitrile	8	REL	100	0.08	Mouse-LD50 - ROUTE: oral; DOSE: 191 mg/kg (RTECS). No toxicity information located. Based on structural similarity to butanenitrile (109-74-0).
542-54-1	4-Methylpentanenitrile	2-Methylpropanenitrile	8	REL	100	0.08	Mouse-LD50 - ROUTE: oral; DOSE: 488 mg/kg (RTECS); working REL assigned on basis of NIOSH REL for structural surrogate 2-methylpropanenitrile (78-82-0).
628-73-9	Hexanenitrile	Butanenitrile	8	REL	100	0.08	Mouse-LD50 - ROUTE: oral; DOSE: 463 mg/kg (RTECS). No toxicity information located although indications are that alkyl nitrile toxicity may decrease with increasing length of akyl chain (Grogan et al. *Chem. Res. Toxicol.* 5(4):548-552, 1992). Screening value based on OEL (NIOSH REL) for butanenitrile (109-74-0).
629-08-3	Heptanenitrile	Butanenitrile	8	REL	100	0.08	No toxicity information located although indications are that alkyl nitrile toxicity may decrease with increasing length of alkyl chain (Grogan et al. *Chem. Res. Toxicol*. 5(4):548-552, 1992). Screening value based on OEL (NIOSH REL) for butanenitrile (109-74-0).
124-12-9	Octanenitrile	Butanenitrile	8	REL	100	0.08	Mouse-LD50 - ROUTE: Oral; DOSE: 1764 mg/kg (RTECS); no toxicity information located although indications are that alkyl nitrile toxicity may decrease with increasing length of akyl chain (Grogan et al. *Chem. Res. Toxicol.* 5(4):548-552, 1992). Screening value based on OEL (NIOSH REL) for butanenitrile (109-74-0).

Table A.9. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALKANE NITRILES						
2243-27-8	Nonanenitrile	Butanenitrile	8	REL	100	0.08	Mouse-LD50 - ROUTE: oral; DOSE: 2059 mg/kg (RTECS); no toxicity information located although indications are that alkyl nitrile toxicity may decrease with increasing length of akyl chain (Grogan et al. *Chem. Res. Toxicol.* 5(4):548-552, 1992). Screening value based on OEL (NIOSH REL) for butanenitrile (109-74-0).
1975-78-6	Decanenitrile	Butanenitrile	8	REL	100	0.08	No toxicity information located although indications are that alkyl nitrile toxicity may decrease with increasing length of akyl chain (Grogan et al. *Chem. Res. Toxicol.* 5(4):548-552, 1992). Screening value based on OEL (NIOSH REL) for butanenitrile (109-74-0).
2244-07-7	Undecanenitrile	Butanenitrile	8	REL	100	0.08	No toxicity information located although indications are that alkyl nitrile toxicity may decrease with increasing length of akyl chain (Grogan et al. *Chem. Res. Toxicol.* 5(4):548-552, 1992).
629-60-7	Tridecanenitrile	Butanenitrile	8	REL	100	0.08	No toxicity information located although indications are that alkyl nitrile toxicity may decrease with increasing length of akyl chain (Grogan et al. *Chem. Res. Toxicol.* 5(4):548-552, 1992).
	Incompletely Identified Alkane Nitriles						
UNI007-01	C7-Nitrile	Butanenitrile	8	REL	100	0.08	No toxicity information located although indications are that alkyl nitrile toxicity may decrease with increasing length of akyl chain (Grogan et al. *Chem. Res. Toxicol.* 5(4):548-552, 1992).
UNI008-01	C8-Nitrile	Butanenitrile	8	REL	100	0.08	No toxicity information located although indications are that alkyl nitrile toxicity may decrease with increasing length of akyl chain (Grogan et al. *Chem. Res. Toxicol.* 5(4):548-552, 1992).
	ALKENE NITRILES						
4786-20-3	2-Butenenitrile	2-Propenenitrile	2	TLV	100	0.02	Screening value based on structural similarity to 2-propenenitrile (107-13-1)

Table A.9. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALKENE NITRILES						
109-75-1	3-Butenenitrile	2-Propenenitrile	2	TLV	100	0.02	Screening value based on structural similarity to 2-propenenitrile (107-13-1)
1615-70-9	2,4-Pentadienenitrile	2-Propenenitrile	2	TLV	100	0.02	Highly toxic when inhaled or ingested (OHM/TADS). Compound has potential to form relatively stable, strongly nucleophilic epoxide due to unsaturation and conjugation with cyano group. ACGIH value for surrogate 2-propenenitrile (107-13-1) used for screening value.
	CYCLOALKANE NITRILES						
5500-21-0	Cyclopropanenitrile	Propanenitrile	6	REL	100	0.06	No toxicity information located. Working TLV based on structural similarity to propanenitrile (107-12-0).
	AROMATIC NITRILES						
100-47-0	Benzonitrile	n.a.	n.a.	n.a.	n.a.	1	Rats-LC50 3.9 mg/l (~850 ppm) (HSDB). Rat-TCLo - ROUTE: inhalation; DOSE: 70 mg/m3/4H/19W intermittent (RTECS).

Table A.10. Amines and Amides

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALIPHATIC AMINES						
6898-69-7	N-(Butylidene)methanamine	N,N-Dimethylmethanamine	5	TLV	100	0.05	No toxicity information located for this compound. Screening Value based on structural similarity to N,N-dimethylmethanamine (75-50-3).
10599-75-4	N-(Pentylidene)methanamine	N,N-Dimethylmethanamine	5	TLV	100	0.05	No toxicity information located for this compound. Screening Value based on structural similarity to N,N-dimethylmethanamine (75-50-3).
22431-09-0	N-(1-Methylbutylidene) methanamine	N,N-Dimethylmethanamine	5	TLV	100	0.05	No toxicity information located for this compound. Screening Value based on structural similarity to N,N-dimethylmethanamine (75-50-3).
1196-92-5	4-Hydroxy-3-methoxybenzyl methanamine	N,N-Dimethylmethanamine	5	TLV	100	0.05	No toxicity information located for this compound. Screening Value based on structural similarity to N,N-dimethylmethanamine (75-50-3).
78-96-6	1-Amino-2-propanol	n.a.	n.a.	n.a.	n.a.	0.2	Little toxicity information located for this compound. RTECS; rat oral LD50 1715 mg/kg (for Cas # 78-96-6), rabbit dermal 1640 µl/kg. Potential reproductive toxicant. Screening Value based on toxicity information, with additional SF of 10 for reproductive effects.
151-18-8	3-Cyanopropanamine	Propanenitrile	6	REL	100	0.06	Toxicity of this compound results from metabolic release of cyanide. (HSDB). Mouse- LD50 - ROUTE: intraperitoneal; DOSE: 1,152 mg/kg (RTECS). Set conservatively, based on cyanide metabolite and margin of exposure and structural similarity to propanenitrile (107-12-0).
6898-74-4	N-Ethylidene-1-butanamine	N-2-Propenyl-2-propen-1-amine	1	WEEL	100	0.01	No toxicity information located for this compound. Screening Value based on N-ethylethanamine (109-89-7; TLV = 5 ppm), N,N-diisopropylamine (108-18-9; TLV = 5 ppm), N-butylbutanamine (111-92-2; WEEL ceiling = 5 ppm), as well as on two unsaturated amines, 2-propenamine (allylamine, 107-11-9; Sweden TWA = 2 ppm) and N-2-propenyl-2-propen-1-amine (diallylamine, 124-02-7; WEEL = 1 ppm). Ciritical effects include irritation and vision.

Table A.10. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALIPHATIC AMINES						
10599-77-6	N-Pentylidene-1-butanamine	N-2-Propenyl-2-propen-1-amine	1	WEEL	100	0.01	No toxicity information located for this compound. Screening Value based on N-ethylethanamine (109-89-7; TLV = 5 ppm), N,N-diisopropylamine (108-18-9; TLV = 5 ppm), N-butylbutanamine (111-92-2; WEEL ceiling = 5 ppm), as well as on two unsaturated amines, 2-propenamine (allylamine, 107-11-9; Sweden TWA = 2 ppm) and N-2-propenyl-2-propen-1-amine (diallylamine, 124-02-7; WEEL = 1 ppm). Critical effects include irritation and vision.
3760-63-2	4-(Dimethylamino)-1-phenyl-1-butanone	N-2-Propenyl-2-propen-1-amine	1	WEEL	100	0.01	No toxicity information located for this compound. Screening Value based on N-ethylethanamine (109-89-7), N,N-disopropylamine (108-18-9; TLV = 5 ppm), N-butylbutanamine (111-92-2; WEEL ceiling = 5 ppm), as well as on two unsaturated amines, 2-propenamine (allylamine, 107-11-9; Sweden TWA = 2 ppm) and N-2-propenyl-2-propen-1-amine (diallylamine, 124-02-7; WEEL = 1 ppm). Critical effect: irritation. These compounds are also potent alkylating agents.
2508-29-4	5-Hydroxy-1-pentanamine	n-Butylamine	5	TLV Ceiling	100	0.05	Screening Value based on structural similarity to n-butylamine (109-73-9). Critical effect: irritation.
124-28-7	N,N-Dimethyl-1-octadecanamine	N,N-Dimethyl-ethanamine	10	UK OES	100	0.1	No toxicity information located. Based on structural similarity to N,N-dimethylethanamine (598-56-1).
	CYCLIC ALIPHATIC AMINES						
1072-44-2	N-Methylaziridine	2-Methylaziridine	2	TLV	100	0.02	Mouse - LC - ROUTE: Inhalation; DOSE: >2 gm/m3/10M (RTECS). Screening Value based on structural similarity to 2-methylaziridine (75-55-8).
2549-67-9	2-Ethylaziridine	2-Methylaziridine	2	TLV	100	0.02	Screening Value based on structural similarity to 2-methylaziridine (75-55-8).
20691-89-8	1-Methyl-4-piperidinemethanol	Piperidine	1	WEEL	100	0.01	Screening Value based on USA WEEL of 1 ppm for piperidine (110-89-4), the parent compound for 1-methyl-4-piperidinemethanol.

Table A.10. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	CYCLIC ALIPHATIC AMINES						
100-97-0	1,3,5,7-Tetra azatri(3.3.1.1(3,7))decane	n.a.	0.524	Norway TWA	10	0.052	Hexamethylenetetramine; rat: TCLo - ROUTE: Inhalation; DOSE: 350 mg/m3/2H/3W intermittent (RTECS). Screening Value based on TCLo for rats, data reported for multiple dose studies (RTECS and HSDB), and the Norway OEL TWA = 3 mg/m3.
	AROMATIC AMINES						
578-54-1	2-Ethylbenzenamine	Methyl aniline	0.5	TLV	100	0.005	Rat oral LD50 1260 mg/kg. Similar to methyl aniline (100-61-8).
	ALIPHATIC AMIDES						
1467-79-4	Dimethylcyanamide	n.a.	n.a.	n.a.	n.a.	8	Rat:LC50 - ROUTE: Inhalation; DOSE: 2500 mg/m3 (800 ppm); mouse: 2800 mg/m3 (900 ppm). (RTECS). Screening Value set on LC50 with a protection factor of 100 for species extrapolation.
123-39-7	N-Methylformamide	n.a.	n.a.	n.a.	n.a.	0.4	Rat-TCLo - ROUTE: Inhalation; DOSE: 400 ppm/6H/2W intermittent (RTECS). Oral LD50s are 2600 and 4000 mg/kg for mouse and rat (RTECS). Screening Value based on TCLo with safety factor of 100 due to short exposure period. Has been shown to cause hepatic and reproductive toxicity in animal studies (HSDB, 2002).
6281-96-5	N-(2-Methylpropyl) formamide	Formamide	10	TLV	100	0.1	Screening Value based on structural similarity to formamide (75-12-7).
871-71-6	N-Butylformamide	Formamide	10	TLV	100	0.1	Screening Value based on structural similarity to formamide (75-12-7).
60-35-5	Acetamide	N,N-Dimethylacetamide	10	TLV	1000	0.01	Acetamide. IARC group 2B (possible carcinogen). Screening Value based on N,N-dimethylacetamide (10). Safety factor of 100 included in light of carcinogen status.
79-16-3	N-Methylacetamide	N,N-Dimethylacetamide	10	TLV	100	0.1	Screening Value set on structural similarity to N,N-dimethylacetamide (127-19-5).
541-35-5	Butanamide	N,N-Dimethylacetamide	10	TLV	100	0.1	Screening Value set on structural similarity to N,N-dimethylacetamide (127-19-5).

Table A.10. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	ALIPHATIC AMIDES						
10264-17-2	N-Hexylbutanamide	N,N-Dimethylacetamide	10	TLV	100	0.1	No toxicity information located. Screening Value based on N,N-dimethylacetamide (127-19-5).
7112-02-9	N-(2-Hydroxyethyl) octanamide	1-Octanol	50	WEEL	100	0.5	Screening Value based on structural similarity to 1-octanol (29063-28-3) and potential for metabolism to corresponding alcohol (WEEL 50-ppm).
1120-07-6	Nonanamide	Nonanal	50	WEEL	100	5	Screening Value based on structural similarity to nonanal and potential for metabolism to this corresponding aldehyde (TLV 50-ppm).
7726-08-1	N-(2-Hydroxyethyl) decanamide	n.a.	n.a.	n.a.	n.a.	5	Screening Value based on structural similarity to corresponding aldehyde and the potential for metabolism to this corresponding aldehyde.
142-78-9	N-(2-Hydroxyethyl) dodecanamide	n.a.	n.a.	n.a.	n.a.	5	Screening Value based on structural similarity to corresponding aldehyde and the potential for metabolism to this corresponding aldehyde.
629-54-9	Hexadecanamide	n.a.	n.a.	n.a.	n.a.	5	Screening Value based on structural similarity to corresponding aldehyde and the potential for metabolism to this corresponding aldehyde.
	CYCLIC ALIPHATIC AMIDES						
616-45-5	2-Pyrrolidinone	1-Methyl-2-pyrrolidinone	10	WEEL	100	0.1	Screening Value based on WEEL for 1-methyl-2-pyrrolidinone (872-50-4).
123-56-8	2,5-Pyrrolidinedione	n.a.	n.a.	n.a.	n.a.	10	Succinimide, rat: LD50 - ROUTE: oral; DOSE: 14 gm/kg (RTECS), Screening Value based on low oral toxicity. Conservative based on margin of exposure.
1121-07-9	1-Methyl-2,5-pyrrolidinedione	n.a.	n.a.	n.a.	n.a.	10	Rat:LD50 - ROUTE: oral; DOSE: >6 gm/kg, (RTECS). Screening Value based on low oral toxicity. Conservative based on margin of exposure.
58467-28-0	3-Ethyl-3-hydroxy-2,5-pyrrolidinedione	n.a.	n.a.	n.a.	n.a.	10	No toxicity information located. Screening Value based on structural similarity to 1-methyl-2,5-pyrrolidione. Conservative based on margin of exposure.
5115-98-0	N-Methyl-3-piperidinecarboxamide	n.a.	n.a.	n.a.	n.a.	1	No toxicity information located on this or closely related compounds. Screening Value set conservatively on basis of author's experience.

Table A.10. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	BENZENAMIDES						
613-93-4	N-Methylbenzamide	Methyl aniline	0.5	TLV	100	0.005	No toxicity information on this compound. Structurally similar to methyl analine (100-61-8).

Table A.11. Nitrous and Nitric Acid Esters and Nitro Compounds

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	NITROUS ACID ESTERS						
624-91-9	Methyl nitrite	n.a.	n.a.	n.a.	n.a.	0.2	Rat-LC50 - ROUTE: inhalation; DOSE: 176 ppm/4H (RTECS); Screening Value proposed on basis of rat LC50 with a safety factor of 100 in light of short exposure time. HSDB: occupational exposure in humans resulted in severe methemoglobinemia. 50 ppm considered upper limit of safety for workers.
109-95-5	Ethyl nitrite	n.a.	n.a.	n.a.	n.a.	0.2	Rat-LC50 - ROUTE: inhalation; DOSE: 160 ppm/4H (RTECS). Screening Value based on LC50 with safety factor of 100 due to short exposure time. HSDB: Can cause methemoglobinemia in humans.
544-16-1	Butyl nitrite	n.a.	n.a.	n.a.	n.a.	0.4	Rat-LC50 - ROUTE: inhalation; DOSE: 420 ppm/4H (RTECS). Screening Value proposed on basis of rat LD50 with a safety factor of 100 in light of short exposure time.
	NITRIC ACID ESTERS						
598-58-3	Methyl nitrate	n.a.	n.a.	n.a.	n.a.	1.3	Rat-LC50 - ROUTE: inhalation; DOSE: 1275 ppm/4H (RTECS); effects-methemoglobinemia; Screening Value based on rat LC50 with a safety factor of 1000 in light of short exposure time.
625-58-1	Ethyl nitrate	n.a.	n.a.	n.a.	n.a.	1.3	Listed as highly toxic to humans via inhalation route (HSDB). Causes cyanosis and methemoglobinemia. Screening Value set on basis of toxicity to humans and similarity to methyl nitrate.
1712-64-7	1-Methylethyl nitrate	n.a.	10	Sweden TWA	10	1	Isopropyl nitrate; 10 ppm Sweden; Screening Value based on structural similarity to methyl nitrate (598-58-3) and Swedish OEL.
543-29-3	2-Methylpropyl nitrate	Propyl nitrate	25	TLV	100	0.25	Screening Value based on structural similarity to propyl nitrate (627-13-4).
926-42-1	2,2-Dimethyl-1-propyl nitrate	Propyl nitrate	25	TLV	100	0.25	Screening Value based on structural similarity to propyl nitrate (627-13-4).
928-45-0	Butyl nitrate	Propyl nitrate	25	TLV	100	0.25	Screening Value based on structural similarity to propyl nitrate (627-13-4).

Table A.11. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	NITRIC ACID ESTERS						
543-87-3	3-Methyl-1-butyl nitrate	Propyl nitrate	25	TLV	100	0.25	LD50: 480 mg/kg intraperitonal mouse. Toxic effect: somnolence. (RTECS) Screening Value based on structural similarity to propyl nitrate (627-13-4).
1002-16-0	Pentyl nitrate	Propyl nitrate	25	TLV	100	0.25	LCLo: 1807 ppm/7 h, inhalation rabbit and mouse. Toxic effects: convulsions, cyanosis, ataxia. (RTECS) Screening Value based on structural similarity to propyl nitrate (627-13-4).
20633-11-8	Hexyl nitrate	Propyl nitrate	25	TLV	100	0.25	Screening Value based on structural similarity to propyl nitrate (627-13-4).
20633-12-9	Heptyl nitrate	Propyl nitrate	25	TLV	100	0.25	Screening Value based on structural similarity to propyl nitrate (627-13-4).
20633-13-0	Nonyl nitrate	Propyl nitrate	25	TLV	100	0.25	Screening Value based on structural similarity to propyl nitrate (627-13-4).
2050-78-4	Decyl nitrate	Propyl nitrate	25	TLV	100	0.25	Screening Value based on structural similarity to propyl nitrate (627-13-4).
	DINITRATE ESTERS						
3457-90-7	1,3-Propanediol, dinitrate	Propylene glycol dinitrate	0.05	TLV	100	0.0005	Screening Value based on close structural similarity to propylene glycol dinitrate (6423-43-4); critical effect: headaches, CVS, CNS, anoxia.
3457-91-8	1,4-Butanediol, dinitrate	Propylene glycol dinitrate	0.05	TLV	100	0.0005	Screening Value based on close structural similarity to propylene glycol dinitrate (6423-43-4); critical effect: headaches, CVS, CNS, anoxia.
3457-92-9	1,5-Pentanediol, dinitrate	Propylene glycol dinitrate	0.05	TLV	100	0.0005	Screening Value based on close structural similarity to propylene glycol dinitrate (6423-43-4); critical effect: headaches, CVS, CNS, anoxia.
624-43-1	1,2,3-Propanetriol, 1-nitrate	Propylene glycol dinitrate	0.05	TLV	100	0.0005	Rat-LD50 - ROUTE: oral; DOSE: 339 mg/kg, cyanosis, respiratory depression (RTECS); Screening Value based on similarity to 1,3-propanediol dinitrate.
623-87-0	1,2,3-Propantriol, 1,3-dinitrate	Propylene glycol dinitrate	0.05	TLV	100	0.0005	Glycerol, 1,3-dinitrate; Rat-LD50 - ROUTE: oral; DOSE: 1065 mg/kg (RTECS); Screening Value based on similarity to 1,3-propanediol dinitrate.

Table A.11. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	Incompletely Identified Nitrates						
UNA003-01	C3-Nitrate	Propyl nitrate	25	TLV	100	0.25	Screening Value based on TWA for propyl nitrate (627-13-4); critical effect: anoxia (methemoglobinemia).
	NITRO COMPOUNDS						
625-76-3	Dinitromethane	Nitromethane	20	TLV	100	0.2	No specific toxicity information located. Low molecular weight nitroparaffin compounds listed as toxic to humans causing headache, nausea, damage to respiratory tract and liver damage (Anonymous, *Information Profiles on Potential Occupational Hazards: Nitroparaffins.* Syracuse Research Corporation, SRC TR 81-617, Contract No. 210-79-0030. 1981). Screening Value based on this and similarity to nitromethane (75-52-5).
517-25-9	Trinitromethane	Nitromethane	20	TLV	100	0.2	RTECS: mammal - unspecified upecies-- LCLo - ROUTE: inhalation; DOSE: 200 mg/m^3 TOXIC EFFECTS: brain and coverings - other degenerative changes; behavioral - convulsions or effect on seizure threshold; lung, thorax, or respiration - structural or functional change in trachea or bronchi. Mouse: LC50 - ROUTE: inhalation; DOSE: 800 mg/m^3/2H; TOXIC EFFECTS: behavioral - general anesthetic; behavioral – ataxia; lung, thorax, or respiration – dyspnea. rat: TDLo - ROUTE: inhalation; DOSE: 120 mg/m^3/2H/9W intermittent; TOXIC EFFECTS: blood - changes in other cell count (unspecified);others – death. Screening Value based on similarity to nitromethane (75-52-5).
1840-42-2	Trinitrofluoromethane	n.a.	n.a.	n.a.	n.a.	10	Mouse-LD50 - ROUTE: intraperitoneal; DOSE: 57300 μg/kg (RTECS). Only toxicity information located was this mouse LD50 in RTECS. Screening Value set conservatively.
600-40-8	1,1-Dinitroethane	Nitroethane	100	TLV	100	1	Screening Value based on similarity to dinitroethane. RTECS: Mouse LD50, ip, 250 mg/kg. This value is comparable to that for nitromethane (RTECS: Mouse LD50, ip, 310 mg/kg.).

Table A.11. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	NITRO COMPOUNDS						
2902-96-7	2-Nitro-1-propanol	2-Nitropropane	10	TLV	100	0.1	Non-mutagenic in several mutagenicity tests (CCRIS database). No other toxicity information located. Screening values based on structural similarity to 2-nitropropane (79-46-9).
594-70-7	2-Nitro-2-methylpropane	2-Nitropropane	10	TLV	100	0.1	Screening Value based on structural similarity to 2-nitropropane (79-46-9).
625-74-1	2-Methyl-1-nitropropane	2-Nitropropane	10	TLV	100	0.1	Screening Value based on structural similarity to 2-nitropropane (79-46-9).
627-05-4	1-Nitrobutane	1-Nitropropane	25	TLV	100	0.25	Rabbit-LDLo - ROUTE: oral; DOSE: 500 mg/kg (RTECS); Screening Value based on structural similarity to 1-nitropropane (108-03-2).
600-24-8	2-Nitrobutane	2-Nitropropane	10	TLV	100	0.1	Based on structural similarity to 2-nitropropane (79-46-9).
27675-36-1	Z-1-Nitropropene	1-Nitropropane	25	TLV	100	0.25	Based on structural similarity to 1-nitropropane (108-03-2).
	NITROSO COMPOUNDS						
865-40-7	Nitrosomethane	Nitromethane	20	TLV	100	0.2	No specific toxicity information located. Nitrosomethane has been shown to coordinate with heme iron in vitro, thus the possibility for forming methemoglobin exists (Stone JR, Marletta MA, *Biochemistry.* 1995 Dec 19; 34(50):16397-403). Screening value based on nitromethane (75-52-5). Critical effect: thyroid.
925-91-7	Nitrosoethane	Nitromethane	20	TLV	100	0.2	Screening Value based on structural similarity to nitromethane (75-52-5). Critical effect: thyroid.
59-89-2	4-Nitrosomorpholine	n.a.	n.a.	n.a.	n.a.	0.005	N-Nitrosomorpholine (NMOR); N-Nitrosomorpholine is carcinogenic in mice; rats; Syrian golden, Chinese and European hamsters; and various fish. (IARC, VOL.: 17 1978 p. 263). IARC 2B carcinogen; Screening Value based on its carcinogenic potential.

Table A.11. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	OXIMES						
107-29-9	Ethanal oxime	n.a.	n.a.	n.a.	n.a.	0.1	RTECS: mouse-LD50 - ROUTE: intraperitoneal; DOSE: 100 mg/kg. Non-mutagenic in Salmonella assay. No other toxicity information located. Screening Value based on intraperitoneal LD50 with a safety factor of 100.
75-17-2	Methanal oxime	n.a.	n.a.	n.a.	n.a.	0.1	Classified as mutagen (RTECS). No other toxicity information available. Screening Value based on mutagenic activity and structural similarity to ethanal oxime.

Table A.12. Heterocyclic Compounds

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
56052-94-9	cis-2-Ethyl-3-propyloxirane	Ethyloxirane	2	WEEL	100	0.02	No toxicity information located. Screening Value based on structural similarity to ethyloxirane (106-88-7) and ethenyloxirane (930-22-3). Epoxides of this type can bind to genetic material and proteins.
53229-39-3	(1-Methylbutyl)oxirane	Ethyloxirane	2	WEEL	100	0.02	No toxicity information located. Screening Value based on structural similarity to ethyloxirane (106-88-7) and ethenyloxirane (930-22-3). Epoxides of this type can bind to genetic material and proteins.
53907-75-8	2-Methyl-2-pentyloxirane	Ethyloxirane	2	WEEL	100	0.02	No toxicity information located. Screening Value based on structural similarity to ethyloxirane (106-88-7) and ethenyloxirane (930-22-3). Epoxides of this type can bind to genetic material and proteins.
1779-19-7	1,3,6-Trioxocane	1,3-Dioxolane	20	TLV	100	0.2	No toxicity information located. Screening Value based on structural similarity to 1,3-dioxolane (646-06-0; TLV = 20 ppm) and 1,4-dioxane (123-91-1; TLV = 20 ppm).
110-00-9	Furan	Furfuryl Alcohol	10	TLV	1000	0.01	2B IARC carcinogen; rat - LC50 - ROUTE: inhalation; DOSE: 3398 ppm/1H (RTECS); mouse-LC50 - ROUTE: Inhalation; DOSE: 120 mg/m3/1H (RTECS); rat-TCLo - ROUTE: Inhalation; DOSE: 5 mg/m3/4H/26W intermittent (RTECS); all furans appear to be bioactive, and lower alkyl furans are significantly absorbed via the lung (Egle and Gochberg, *Am. Indust. Hyg. Assoc. J.* 40(10):866-869, 1979.) Screening value based on furfuryl alcohol (98-00-0), with additional factor of 10 for 2B carcinogen.
534-22-5	2-Methylfuran	Furfuryl Alcohol	10	TLV	1000	0.01	Rat-LC50 - ROUTE: inhalation; DOSE: 500 ppm/4H (RTECS); TCLo - ROUTE: inhalation; DOSE: 160 ppm/6H/14D intermittent (RTECS); 2-methylfuran has a lower LC50 in the rat than the unsubstituted parent compound; thus, screening value has additional factor of 10 applied.
4229-91-8	2-Propylfuran	Furfuryl Alcohol	10	TLV	1000	0.01	No toxicity information located. Low molecular weight 2-alkyl substitution indicates potential for significant pulmonary absorption. Screening Value set conservatively.

Table A.12. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
3777-69-3	2-Pentylfuran	Furfuryl Alcohol	10	TLV	1000	0.01	No toxicity information located. Low molecular weight 2-alkyl substitution indicates potential for significant pulmonary absorption. Screening Value set conservatively.
3777-71-7	2-Heptylfuran	Furfuryl Alcohol	10	TLV	100	0.1	No toxicity information located. Higher molecular weight 2-alkyl substitution relative to three preceding substituted furans indicates lower potential for pulmonary absorption. Screening Value set conservatively. SF decreased by 10 due to low potential for pulmonary absorption.
625-86-5	2,5-Dimethylfuran	Furfuryl Alcohol	10	TLV	1000	0.01	No toxicity information located. Low molecular weight 2,5-alkyl substitution indicates potential for significant pulmonary absorption. Screening Value set conservatively.
1703-52-2	2-Ethyl-5-methylfuran	Furfuryl Alcohol	10	TLV	1000	0.01	No toxicity information located. Low molecular weight 2-alkyl substitution indicates potential for significant pulmonary absorption. Screening Value set conservatively.
4179-38-8	2-Octylfuran	Furfuryl Alcohol	10	TLV	1000	0.01	No toxicity information located. Higher molecular weight 2,5-alkyl substitution relative to three preceding substituted furans indicates lower potential for pulmonary absorption. Screening Value set conservatively.
51595-87-0	2-(2-Methyl-6-oxoheptyl) furan	Furfuryl Alcohol	10	TLV	1000	0.01	No toxicity information located for this compound. Relatively high MW and branched chain indicate that this compound will undergo limited pulmonary absorption. Screening Value set conservatively.
717-21-5	2-(3-Oxo-3-phenylprop-1-enyl) furan	Furfuryl Alcohol	10	TLV	1000	0.01	In addition to containing the furan moiety, this compound is an alpha-beta unsaturated ketone, a class of compounds frequently found to be bioactive. There is no specific toxicity information on this compound; thus, the Screening Value is set conservatively.
1191-99-7	2,3-Dihydrofuran	Tetrahydrofuran	50	TLV	100	0.5	No toxicity information located for this compound. Screening Value based on OEL for tetrahydrofuran (109-99-9).

Table A.12. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
34314-82-4	3-(1,1-Dimethylethyl)-2,3-dihydrofuran	Tetrahydrofuran	50	TLV	100	0.5	No toxicity information located for this compound. Screening Value based on OEL for tetrahydrofuran (109-99-9).
34379-54-9	4-(1-Methylpropyl)-2,3-dihydrofuran	Tetrahydrofuran	50	TLV	100	0.5	No toxicity information located for this compound. Screening Value based on OEL for tetrahydrofuran (109-99-9).
1708-29-8	2,5-Dihydrofuran	Tetrahydrofuran	50	TLV	100	0.5	Rat: TCLo - ROUTE: inhalation; DOSE: 1250 ppm/6H/4W intermittent (RTECS); Screening Value based on OEL for tetrahydrofuran (109-99-9).
96-47-9	2-Methyltetrahydrofuran	Tetrahydrofuran	50	TLV	100	0.5	RTECS: rat-LC50 - 6000 ppm/4H. Screening Value based on OEL for tetrahydrofuran (109-99-9).
1004-29-1	2-Butyltetrahydrofuran	Tetrahydrofuran	50	TLV	100	0.5	No toxicity information located. Screening Value based on parent compound, tetrahydrofuran (109-99-9).
41239-48-9	2,5-Diethyltetrahydrofuran	Tetrahydrofuran	50	TLV	100	0.5	Rat-LD50 - ROUTE: oral; DOSE: 3400 mg/kg (RTECS); Screening Value based on parent compound, tetrahydrofuran (109-99-9).
4457-62-9	2,5-Dipropyltetrahydrofuran	Tetrahydrofuran	50	TLV	100	0.5	Rat-LD50 - ROUTE: oral; DOSE: 3400 mg/kg (RTECS); Screening Value based on parent compound, tetrahydrofuran (109-99-9).
39168-02-0	trans-2,4-Dimethyl tetrahydrofuran	Tetrahydrofuran	50	TLV	100	0.5	Rat-LD50 - ROUTE: oral; DOSE: 3400 mg/kg (RTECS); Screening Value based on parent compound, tetrahydrofuran (109-99-9).
96-48-0	Dihydro-2(3H)-furanone	n.a.	n.a.	n.a.	n.a.	75	Rat-LC50 - ROUTE: Inhalation; DOSE: >5100 mg/m3/4H (RTECS); rat-TCLo - ROUTE: Inhalation; DOSE: 5030 ug/m3/24H/17W continuous (RTECS); Screening Value based on high LC50, plus known exposure of individuals working with printer's inks (HSDB).
108-29-2	5-Methyldihydro-2(3H)-furanone	n.a.	n.a.	n.a.	n.a.	75	Mouse-TCLo - ROUTE: inhalation; DOSE: 1 gm/m3/7H/92D intermittent (RTECS). Screening Value based on high TCLo.
695-06-7	5-Ethyldihydro-2(3H)-furanone	n.a.	n.a.	n.a.	n.a.	5	Rat-LD50 - ROUTE: oral; DOSE: >5 gm/kg (RTECS). Screening value based on low oral toxicity.
105-21-5	5-Propyldihydro-2(3H)-furanone	n.a.	n.a.	n.a.	n.a.	5	Rat-LD50 - ROUTE: oral; DOSE: >5 gm/kg (RTECS); Screening value based on low oral toxicity.

Table A.12. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
104-50-7	5-Butyldihydro-2(3H)-furanone	n.a.	n.a.	n.a.	n.a.	5	Rat-LD50 - ROUTE: oral; DOSE: 4400 mg/kg (RTECS). Screening value based on low oral toxicity.
706-14-9	5-Hexyldihydro-2(3H)-furanone	5-Butyldihydro-2(3H)-furanone	n.a.	n.a.	n.a.	5	No LD50 or LC50 data in RTECS. Screening Value based on structural similarity to 5-butyldihydro-2(3H)-furanone (104-50-7), which has a low oral toxicity.
104-67-6	5-Heptyldihydro-2(3H)-furanone	n.a.	n.a.	n.a.	n.a.	15	Rat-LD50 - ROUTE: oral; DOSE: 18500 mg/kg. Screening value based on low oral toxicity.
5145-01-7	3,5-Dimethyldihydro-2(3H)-furanone	n.a.	n.a.	n.a.	n.a.	0.5	No toxicity data located. Screening Value based on structural similarity to other furanones. With SF of 10 added.
13861-97-7	4,4-Dimethyldihydro-2(3H)-furanone	n.a.	n.a.	n.a.	n.a.	0.5	No toxicity data located. Screening Value based on structural similarity to other furanones. With SF of 10 added.
1073-11-6	5-Ethenyldihydro-5-methyl-2(3H)-furanone	n.a.	n.a.	n.a.	n.a.	0.5	No toxicity data located. Screening Value based on structural similarity to other furanones. With SF of 10 added.
2865-82-9	5-Ethyldihydro-5-methyl-2(3H)-furanone	n.a.	n.a.	n.a.	n.a.	0.5	No toxicity data located. Screening Value based on structural similarity to other furanones. With SF of 10 added.
104-61-0	5-Pentyldihydro-2(3H)-furanone	n.a.	n.a.	n.a.	n.a.	0.5	Rat-LD50 - ROUTE: oral; DOSE: 6600 mg/kg (RTECS). Screening Value based on LD50 and structural similarity to other furanones.
108-30-5	Dihydro-2,5-furandione	2,5-Furanedione	0.25	PEL	100	0.0025	Succinic anhydride. Rat-LD50 - ROUTE: oral; DOSE: 1510 mg/kg (RTECS); severe irritant. irritancy.
1192-51-4	3-Methyl-2,4(3H,5H)-furandione	2,5-Furanedione	0.25	PEL	100	0.0025	No toxicity information located. Screening Value based on 2,5-furanone (108-30-5).
54774-28-6	trans-5-Methyl tetrahydrofuranmethanol	Tetrahydro-2-furanmethanol	2	WEEL	100	0.02	Based on structural similarity to tetrathydro-2-furanmethanol (97-99-4).
16778-26-0	3a,4,5,6-Tetrahydro-3a,6,6-trimethylbenzofuranone	Tetrahydrofuran	50	TLV	100	0.5	No toxicity information available. Screening Value based on structural similarity to tetrahydrofuran (109-99-9).
31681-26-2	α-Propyl-2-furan acetaldehyde	Tetrahydro-2-furanmethanol	2	WEEL	100	0.02	Based on structural similarity to tetrahydro-2-furanmethanol (97-99-4).

Table A.12. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
766-15-4	4,4-Dimethyl-1,3-dioxane	1,4-Dioxane	20	TLV	1000	0.02	RTECS: Rat-LCLo, 8000 ppm/4H; Mus LDlo, oral, 1 gm/kg; rat LD50, oral, 3730 µL/kg; rabbit LD50, skin, 3540 µL/kg; reproductive toxicity-rat TCLo, 10 µg/m3/24H/dy (2 ppm/24H/day) for 16W, Estrus cycle disruption and fetal death (Russian study). Screening value based 1,4-dioxane with an additional SF of 10 for structural differences. NIOSH considers 1,4-dioxane to be a potential carcinogen.
20192-66-9	trans-Hexahydro-1,3-benzodioxol-2-one	1,4-Dioxane	20	TLV	1000	0.02	No toxicity information located for this or closely related compound. Screening value based 1,4-Dioxane with an additional SF of 10 for structural differences. NIOSH considers 1,4-dioxane to be a potential carcinogen.
1713-33-3	1-Methyl-7-oxabicyclo[4.1.0]heptane	n.a.	n.a.	n.a.	n.a.	0.05	No toxicity information available. Screening Value based on general information regarding the potential for mutagenicity and genetic toxicity of epoxides.
74793-02-5	2,2-Bioxepane	n.a.	n.a.	n.a.	n.a.	0.05	No toxicity information available. Screening Value based on general information regarding the potential for mutagenicity and genetic toxicity of epoxides.
100-73-2	3,4-Dihydro-2-carboxaldehyde-2H-pyran	n.a.	n.a.	n.a.	n.a.	1.9	Rat-LC50 - ROUTE: inhalation; DOSE: 3225 ppm/4H (RTECS); rat-TCLo - ROUTE: Inhalation; DOSE: 194 ppm/6H/9D intermittent (RTECS). Safety factor of 100 applied to TCLo for rat inhalation.
1927-69-1	Tetrahydro-2-(1,1-Dimethylethoxy)-2H-pyran	3,4-Dihydro-2-carboxaldehyde-2H-pyran	n.a.	n.a.	n.a.	0.19	Screening Value based on structural similarity to 3,4-Dihydro-2-carboxaldehyde-2H-pyran (100-73-2). With an additional SF of 10 for surrogate.
24405-16-1	Tetrahydro-5,6-dimethyl-2H-pyran-2-one	Tetrahydro-6-hexyl-2H-pyran-2-one	n.a.	n.a.	n.a.	1	No specific toxicity information located. However, a search of toxicological and biomedical databases indicates that other pyran derivatives have been shown to be biologically active (i.e., DNA-binding, potential chemotherapeutic agents, etc.). Screening values are set conservatively based on the above information.

Table A.12. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
2610-95-9	Tetrahydro-6,6-dimethyl-2H-pyran-2-one	Tetrahydro-6-hexyl-2H-pyran-2-one	n.a.	n.a.	n.a.	1	No specific toxicity information located. However, a search of toxicological and biomedica databases indicates that other pyran derivatives have been shown to be biologically active (i.e., DNA-binding, potential chemotherapeutic agents, etc.). Screening values are set conservatively based on the above information.
23462-75-1	Dihydro-2H-pyran-3(4H)-one	Tetrahydro-6-hexyl-2H-pyran-2-one	n.a.	n.a.	n.a.	1	No specific toxicity information located. However, a search of toxicological and biomedica databases indicates that other pyran derivatives have been shown to be biologically active (i.e., DNA-binding, potential chemotherapeutic agents, etc.). Screening values are set conservatively based on the above information.
91894-15-4	4-Methoxy-6-methyl-6,7-dihydro-4H-furo[3,2-c]pyran	Tetrahydro-6-hexyl-2H-pyran-2-one	n.a.	n.a.	n.a.	1	No specific toxicity information located. However, a search of toxicological and biomedica databases indicates that other pyran derivatives have been shown to be biologically active (i.e., DNA-binding, potential chemotherapeutic agents, etc.). Screening values are set conservatively based on the above information.
693-98-1	2-Methyl-1H-imidazole	n.a.	n.a.	n.a.	n.a.	0.1	No toxicity data for 2-methyl-1H-imidazole. Very little toxicity data for 1H-imidazole (288-32-4). Rat-LD50 - ROUTE: oral; DOSE: 220 mg/kg . Mallinkrodt Baker, INC. MSDS identifies 1H-imidazole as "HARMFUL IF SWALLOWED OR INHALED." Screening Value based on this information.
948-65-2	2-Phenyl-1H-indole	n.a.	n.a.	n.a.	n.a.	0.1	Very little toxicity information. Rat-LD50 - ROUTE: oral; DOSE: >6 gm/kg (RTECS). Screening value based on toxicity information for base compound, indole (120-72-9). RTECS: low oral toxicity, Rat LD50 1 gm/kg. Classified by RTECS as equivocal tumorigen in animals (leukemia, respiratory tumors). Screening Value set conservatively.

Table A.12. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
109-97-7	1H-Pyrrole	n.a.	n.a.	n.a.	n.a.	0.03	Rat-LDLo - ROUTE: Oral; DOSE: 147 mg/kg (RTECS); very little toxicity information available. Screening Value based on fact that the rat, oral LD50 for 1H-pyrrole is less than for the preceding 2-phenyl-1H-indole (>6 gm/kg).
625-84-3	2,5-Dimethyl-1H-pyrrole	n.a.	n.a.	n.a.	n.a.	0.01	Very little toxicity information. Rat-LD50 -LD50 - ROUTE: Oral; DOSE: 59 mg/kg (RTECS). Oral LD50 less than for the unsubstituted 1H-pyrrole. Screening Value proposed accordingly.
699-22-9	1-Pentyl-1H-pyrrole	n.a.	n.a.	n.a.	n.a.	0.1	No toxicity information located. Screening Value based on structural similarity to 2,5-dimethyl-1H-pyrrole.
59983-39-0	2-(Methoxymethyl)-1-pyrrolidinamine	n.a.	n.a.	n.a.	n.a.	0.1	No toxicity information located. Screening Value set conservatively.
3760-54-1	1-Pyrrolidine carboxylaldehyde	n.a.	n.a.	n.a.	n.a.	0.1	No toxicity information located. Screening Value set conservatively.
51953-17-4	4(3H)-Pyrimidinone	n.a.	n.a.	n.a.	n.a.	0.1	No toxicity information located. Screening Value set conservatively.
4562-27-0	4(1H)-Pyrimidinone	n.a.	n.a.	n.a.	n.a.	0.1	No toxicity information located. Screening Value set conservatively.
UHC000-09	Methylpyridine	2-Methylpyridine 3-Methylpyridine 4-Methylpyridine	2 2 2	WEEL WEEL WEEL	100	0.02	Screening Value set on basis of structural similarity to methylpyridines.
100-71-0	2-Ethylpyridine	Pyridine	5	TLV	100	0.05	Screening Value set on basis of structural similarity to pyridine (110-86-1).
108-47-4	2,4-Dimethylpyridine	2-Methylpyridine 3-Methylpyridine 4-Methylpyridine	2 2 2	WEEL WEEL WEEL	100	0.02	Rat-LD50 - ROUTE: oral; DOSE: 200 mg/kg (RTECS). Screening Value based on rat LD50 and structural similarity to methylpyridines.
589-93-5	2,5-Dimethylpyridine	2-Methylpyridine 3-Methylpyridine 4-Methylpyridine	2 2 2	WEEL WEEL WEEL	100	0.02	Rat-LD50 - ROUTE: oral; DOSE: 800 mg/kg (RTECS); Screening Value based on rat LD50 and structural similarity to methylpyridines.
108-48-5	2,6-Dimethylpyridine	2-Methylpyridine 3-Methylpyridine 4-Methylpyridine	2 2 2	WEEL WEEL WEEL	100	0.02	Rat-LCLo - ROUTE: inhalation; DOSE: 7500 ppm/1H (RTECS); Screening Value based on LCLo and structural similarity to methylpyridines.

Table A.12. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
583-58-4	3,4-Dimethylpyridine	2-Methylpyridine 3-Methylpyridine 4-Methylpyridine	2 2 2	WEEL WEEL WEEL	100	0.02	Rat-LCLo - ROUTE: Inhalation; DOSE: 500 ppm/4H (RTECS); Screening Value based on LCLo and structural similarity to methylpyridines.
591-22-0	3,5-Dimethylpyridine	2-Methylpyridine 3-Methylpyridine 4-Methylpyridine	2 2 2	WEEL WEEL WEEL	100	0.02	No toxicity information located. Screening Value based on structural similarity to methylpyridines.
104-90-5	5-Ethyl-2-methylpyridine	2-Methylpyridine 3-Methylpyridine 4-Methylpyridine	2 2 2	WEEL WEEL WEEL	100	0.02	Rat-LC50 - ROUTE: inhalation; DOSE: 540 ppm/4H (RTECS); severe irritant (RTECS). Screening Value based on LC50, irritation and structural similarity to methylpyridines.
1462-84-6	2,3,6-Trimethylpyridine	2-Methylpyridine 3-Methylpyridine 4-Methylpyridine	2 2 2	WEEL WEEL WEEL	100	0.02	No toxicity information available. Screening Value based on structural similarity to methylpyridines.
694-05-3	1,2,3,6-Tetrahydropyridine	Pyridine	5	TLV	100	0.05	No toxicity information available. Screening Value based on structural similarity to pyridine (110-86-1).
289-95-2	Pyrimidine	n.a.	n.a.	n.a.	n.a.	3	Mouse-LD50 - ROUTE: Intraperitoneal; DOSE: 3310 mg/kg (RTECS). Screening Value set conservatively based on LD50. With SF of 1000 and assume mg/kg similar to ppm.
3438-46-8	4-Methylpyrimidine	Pyrimidine	n.a.	n.a.	n.a.	0.3	No toxicity information located. Screening Value based on structural similarity to pyrimidine (289-95-2) and its toxicity.
290-37-9	Pyrazine	n.a.	n.a.	n.a.	n.a.	2	Mouse-LD50 - ROUTE: intraperitoneal; DOSE: 2730 mg/kg (RTECS); Screening Value based on relatively low toxicity indicated by mouse LD50.
109-08-0	Methylpyrazine	n.a.	n.a.	n.a.	n.a.	1	Rat-LD50 - ROUTE: oral; DOSE: 1800 mg/kg (RTECS); Screening Value based on relatively low toxicity indicated by rat oral LD50.
13925-00-3	Ethylpyrazine	Methylpyrazine	n.a.	n.a.	n.a.	0.1	Non-mutagenic in Salmonella assay (CCRIS); no other toxicity information located; Screening Value based on structural similarity to methylpyrazine (109-08-0).
5910-89-4	2,3-Dimethylpyrazine	n.a.	n.a.	n.a.	n.a.	0.5	Rat-LD50 - ROUTE: oral; DOSE: 613 mg/kg (RTECS); Screening Value based on rat, oral, LD50.
123-32-0	2,5-Dimethylpyrazine	n.a.	n.a.	n.a.	n.a.	1	Rat-LD50 - ROUTE: oral; DOSE: 1020 mg/kg (RTECS); Screening Value based on rat, oral, LD50.

Table A.12. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
18433-98-2	2,5-Dimethyl-3-(3-methylbutyl)pyrazine	2-Methylpyridine 3-Methylpyridine 4-Methylpyridine	2 2 2	WEEL WEEL WEEL	100	0.02	No toxicity information located. Screening Value based structural similarity to methylpyrazines and their toxicological data.
288-88-0	1H-1,2,4-Triazole	n.a.	n.a.	n.a.	n.a.	1	Rat-LD50 - ROUTE: oral; DOSE: 1750 mg/kg (RTECS); Rat-TDLo - ROUTE: oral; DOSE: 364 mg/kg/26W intermittent (RTECS); Screening Value based on rat oral LD50 and TDlo.
42786-06-1	3-Amino-4-ethyl-4H-1,2,4-triazole	n.a.	n.a.	n.a.	n.a.	1	No toxicity information located. For 1,2,4-triazole: rat LD50, oral, 1350 mg/kg. Rat TDlo 354 mg/kg, 26 weeks. Screening Value based on these data.
930-36-9	1-Methyl-1H-pyrazole	3-Methyl-1H-pyrazole	n.a.	n.a.	n.a.	0.02	No toxicity information located. Screening Value based on structural similarity 3-methyl-1H-pyrazole (1453-58-3).
1568-20-3	5-Methyl-4,5-dihydro-1H-pyrazole	n.a.	n.a.	n.a.	n.a.	0.02	No toxicity information located. Screening Value based on structural similarity to 4,5-dihydro-1,5-dimethyl-1H-pyrazole.
5775-96-2	4,5-Dihydro-1,5-dimethyl-1H-pyrazole	n.a.	n.a.	n.a.	n.a.	0.2	Mouse-LD50 - ROUTE: intravenous; DOSE: 180 mg/kg (RTECS); Screening Value based on mouse, iv, LD50.
28019-94-5	4,5-Dimethyl-4,5-dihydro-1H-pyrazole	4,5-Dihydro-1,5-dimethyl-1H-pyrazole	n.a.	n.a.	n.a.	0.02	No toxicity information located. Screening Value based on structural similarity to 4,5-dihydro-1,5-dimethyl-1H-pyrazole (5775-96-2).
75011-90-4	5-Propyl-4,5-dihydro-1H-pyrazole	4,5-Dihydro-1,5-dimethyl-1H-pyrazole	n.a.	n.a.	n.a.	0.02	No toxicity information located. Screening Value based on structural similarity to 4,5-dihydro-1,5-dimethyl-1H-pyrazole (5775-96-2).
1120-64-5	2-Methyl-4,5-dihydrooxazole	Pyrazole	n.a.	n.a.	n.a.	0.5	No toxicity information located. Screening Value based on 1H pyrazole (67-51-6); >500 mg/kg oral-rat LD; 1060 mg/kg oral-mouse LD50.
53833-32-2	2-n-Propyl-4,5-dimethyloxazole	Pyrazole	n.a.	n.a.	n.a.	0.5	No toxicity information located. Screening Value based on 1H pyrazole (67-51-6); >500 mg/kg oral-rat LD; 1060 mg/kg oral-mouse LD50.
55956-20-2	5-Methyl-3-(2-propenyl)-2-oxazolidinone	Pyrazole	n.a.	n.a.	n.a.	0.5	No toxicity information located. Screening Value based on 1H pyrazole (67-51-6); >500 mg/kg oral-rat LD; 1060 mg/kg oral-mouse LD50.
288-47-1	Thiazole	n.a.	n.a.	n.a.	n.a.	0.1	Mouse-LD50 - ROUTE: oral; DOSE: 983 mg/kg (RTECS); Screening Value based on LD50.

Table A.12. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
288-16-4	Isothiazole	Thiazole	n.a.	n.a.	n.a.	0.01	No toxicity information located. Screening Value based on structural similarity to thiazole (288-47-1).
95-16-9	Benzothiazole	n.a.	n.a.	n.a.	n.a.	1	Rat-LDLo - ROUTE: intraperitoneal; DOSE: 1 gm/kg (RTECS); this LDlo is indicative of low toxicity - Screening Value based on rat LDlo.
	Incompletely Identified Heterocyclics						
UHC000-13	C2-Pyridine	Pyridine	5	TLV	100	0.05	Based on structural similarity to pyridine (110-86-1) and ethyl pyridine.
UHC000-05	C3-Pyridine	Pyridine	5	TLV	100	0.05	Based on structural similarity to pyridine (110-86-1) and ethyl pyridine.
UHC000-07	C4-Piperidine	Piperidine	1	TLV	100	0.01	Based on structural similarity to piperidine (110-89-4) (ACGIH WEEL 1 ppm).
UHC000-10	C2-Pyrrolidine	n.a.	n.a.	n.a.	n.a.	0.4	Mouse-LC50 - ROUTE: inhalation; DOSE: 1300 mg/m3/2H (400 ppm) (RTECS) for pyrrolidine. Screening Value based on mouse LC50 for pyrrolidinone with safety factor of 1000 for short exposure time.
UHC000-06	C4-2-Pyrrolidinone	1-Methyl-2-pyrrolidonone	100	German MAK	100	1	Based on structural similarity to 1-methyl-2-pyrrolidonone (872-50-4) German MAK.

Table A.13. Sulfur Containing Compounds

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	SULFIDES						
463-58-1	Carbonyl sulfide	n.a.	n.a.	n.a.	n.a.	1	Rat-LC50 - ROUTE: inhalation; DOSE: 2270 ppm/4H (RTECS); Screening Value based on rat LC50 with a safety factor of 1000 due to short exposure time. Toxicity likely mediated through hydrogen sulfide (7783-06-4) metabolite, TLV of 10 ppm. Screening value conservative.
UIN000-01	Sulfur oxides (SOx)	Sulfur dioxide	2	TLV	100	0.02	2 ppm is the ACGIH TWA for sulfur dioxide (7446-09-5).
	THIOLS						
1679-08-9	2,2-Dimethyl-1-propanethiol	Propanethiol	n.a.	n.a.	n.a.	7.3	No toxicity information located. Parent compound - propanethiol (107-03-9): LC50 - ROUTE: inhalation; DOSE: 7300 ppm/4H (RTECS). Screening Value based on this LC50 with safety factor of 1000.
	SULFONAMIDES						
3622-84-2	N-Butylbenzenesulfonamide	n.a.	n.a.	n.a.	n.a.	0.015	This compound has been shown to be neurotoxic in rabbits by inducing a spastic myelopathy (*Acta Neuropathologica* 81(3):235-241, 1991). Rat-LCLo - ROUTE: inhalation; DOSE: 385 mg/m3/4H (RTECS). Rat-TCLo - ROUTE: inhalation; DOSE: 1500 ug/m3/17W intermittent (RTECS). Screening value based on Rat TCLo with a safety factor of 10. Russian STEL (1993) 0.5 mg/m^3.
80-39-7	N-Ethyl-N-methylbenzene sulfonamide	N-Butylbenzene-sulfonamide	n.a.	n.a.	n.a.	0.0015	No toxicity information located. Screening Value based on structural similarity to N-butylbenzenesulfonamide (3622-84-2). With an additional SF of 10 for the surrogate.
7250-80-8	N-Hexylbenzenesulfonamide	N-Butylbenzene-sulfonamide	n.a.	n.a.	n.a.	0.0015	No toxicity information located. Screening Value based on structural similarity to N-butylbenzenesulfonamide (3622-84-2).With an additional SF of 10 for the surrogate.
	Incompletely Identified Sulfonamides						
USA000-02	C6-Benzenesulfonamide	N-Butylbenzene-sulfonamide	n.a.	n.a.	n.a.	0.0015	No toxicity information located. Screening Value based on structural similarity to N-butylbenzenesulfonamide (3622-84-2). With an additional SF of 10 for the surrogate.

Table A.14. Silicon Containing Compounds

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	SILANES, SILOXANES, and SILANOLS						
1112-39-6	Dimethoxydimethylsilane	Trimethylsilanol	n.a.	n.a.	n.a.	5	No toxicity information located. Structural similarity to trimethylsilanol (1066-40-6) basis for Screening Value.
107-51-7	Octamethyltrisiloxane	Octamethyl-cyclotetrasiloxane	n.a.	n.a.	n.a.	3	Siloxanes generally have a low order of toxicity (HSDB for Octamethylcyclotetrasiloxane). Surrogate, octamethylcyclotetrasiloxane (556-67-2), used. Rat-TCLo - inhalation, 300 ppm/6H/13W; TDlo 70 ppm/6H/4W (RTECS). Screening Value based on TCLo with safety factor of 100. Dow Corning Corp has set a company guide for octamethyltrisiloxane of 200 ppm.
141-62-8	Decamethyltetrasiloxane	Octamethyl-cyclotetrasiloxane	n.a.	n.a.	n.a.	3	Siloxanes generally have a low order of toxicity (HSDB for Octamethylcyclotetrasiloxane). Surrogate, octamethylcyclotetrasiloxane (556-67-2), used. Rat-TCLo - Inhalation, 300 ppm/6H/13W; TDlo 70 ppm/6H/4W (RTECS). Screening Value based on TCLo with safety factor of 100.
1066-40-6	Trimethylsilanol	n.a.	n.a.	n.a.	n.a.	5	Siloxanes generally have a low order of toxicity. No evidence for clastogenic activity noted when rats dosed at very high levels. No evidence for irritancy of vapors. (HSDB for polydimethylsiloxanes). Screening Value set conservatively.
541-05-9	Hexamethylcyclotrisiloxane	Hexamethyldisiloxane	n.a.	n.a.	n.a.	4.4	Siloxanes generally have a low order of toxicity (HSDB for Octamethylcyclotetrasiloxane). Hexamethyldisiloxane (107-46-0) used as surrogate. When inhaled at 4400 ppm for 19-26 days, it caused slight depression in rat and guinea pig, with a very slight increase in rat liver and kidney weights. (Clayton, G. D. and F. E. Clayton [eds.]. *Patty's Industrial Hygiene and Toxicology*: Volume 2A, 2B, 2C; *Toxicology*. 3rd Ed. New York: John Wiley Sons, 1981-1982, p. 2400) (HSDB for hexamethyldisiloxane [107-46-0]). Screening Value based on this study with a safety factor of 1000 for species differences and surrogate use.

Table A.14. (contd)

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	SILANES, SILOXANES, and SILANOLS						
556-67-2	Octamethylcyclotetrasiloxane	Octamethyl-cyclotetrasiloxane	n.a.	n.a.	n.a.	3	Siloxanes generally have a low order of toxicity (HSDB for Octamethylcyclotetrasiloxane). Rat-TCLo - Inhalation, 300 ppm/6H/13W; TDlo 70 ppm/6H/4W (RTECS). Screening Value based on TCLo with safety factor of 100.
	SILANE ESTERS						
3789-85-3	Trimethylsilyl ester of 2-(trimethylsilyloxy)benzoic acid	Tetraethoxysilane	25	TLV	100	0.25	No toxicity information located. An ACGIH TLV-TWA of 25 ppm was found for tetraethoxysilane (78-10-4). Although this compound is much lower in molecular weight and is only a surrogate for a likely fragment of this compound, the use of 2.5 ppm for the Screening Value with an additional SF of 10 for surrogate use is considered to be adequately conservative.
	OTHER SILICON COMPOUNDS						
USI000-05	Trimethylsilyl ester of methoxybenzoic acid	Tetraethoxysilane	25	TLV	100	0.25	No toxicity information located. An ACGIH TLV-TWA of 25 ppm was found for tetraethoxysilane (78-10-4). Although this compound is much lower in molecular weight and is only a surrogate for a likely fragment of this compound, the use of 2.5 ppm for the Screening Value with an additional SF of 10 for surrogate use is considered to be adequately conservative.

Table A.15. Cyanates, Isocyanates, and Peroxides

CAS or TWINS Number	Chemical	Surrogate			Safety Factor	Screening Value (ppm)	Comments
		Chemical	OEL (ppm)	OEL Source			
	CYANATES and ISOCYANATES						
420-05-3	Cyanic acid	Hydrogen cyanide	4.7	TLV	100	0.047	No toxicity information located. State of South Carolina has set a MAC of 500 µg/m3 (0.28 ppm). Screening Value based on structural similarity to hydrogen cyanide.
75-13-8	Isocyanic acid	n.a.	n.a.	n.a.	n.a.	0.13	No information located. Screening Value based on information for n-butyl isocyanate - rat-inhalation-TDlo, 23.5 mg/m^3 (13.4 ppm); 4H (Pauluhn, J., Eben, A., and Kimmerle, *G., Exp Pathol (Jena);* 40 (4). 1990. 197-202).
	PEROXIDES						
3031-73-0	Methyl hydroperoxide	Hydrogen peroxide	1	TLV	100	0.01	No toxicity information located. Screening Value based on oxidative properties of hydrogen peroxide, which has a TLV of 1 ppm.
3031-74-1	Ethyl hydroperoxide	Hydrogen peroxide	1	TLV	100	0.01	No toxicity information located. Screening Value based on oxidative properties of hydrogen peroxide, which has a TLV of 1 ppm.
484678-32-2	Methyl peroxynitrite	n.a.	n.a.	n.a.	n.a.	0.01	No toxicity information located. Screening Value based on oxidative properties of peroxynitrites; isobutyl nitrite ACGIH TLV 1 ppm.
215229-01-9	Ethyl peroxynitrite	n.a.	n.a.	n.a.	n.a.	0.01	No toxicity information located. Screening Value based on oxidative properties of peroxynitrites; isobutyl nitrite ACGIH TLV 1 ppm.
42829-59-4	Methyl peroxynitrate	Nitrogen dioxide	3	TLV	100	0.03	No toxicity information located. Screening Value based on ACGIH TLV-TWA for nitrogen dioxide (3 ppm). Critical effects: irritation.
64160-40-3	Ethyl peroxynitrate	Nitrogen dioxide	3	TLV	100	0.03	No toxicity information located. Screening Value based on ACGIH TLV-TWA for nitrogen dioxide (3 ppm). Critical effects: irritation.

Table A.16. Maximum Headspace Concentrations and Screening Values

CAS or TWINS Number	Chemical	Max. Conc. (ppm)	Screening Value (ppm)
1002-16-0	Pentyl nitrate	0.16	0.25
1002-84-2	Pentadecanoic acid	0.23	1
1004-29-1	2-Butyltetrahydrofuran	0.037	0.5
100-47-0	Benzonitrile	0.016	1
10061-01-5	Z-1,3-Dichloropropene	**0.0092**	0.001
10061-02-6	E-1,3-Dichloropropene	**0.010**	0.001
100-71-0	2-Ethylpyridine	0.0023	0.05
100-73-2	3,4-Dihydro-2-carboxaldehyde-2H-pyran	0.0016	1.9
1009-61-6	bis-1,1'-(1,4-Phenylene)ethanone	0.00041	0.1
100-97-0	1,3,5,7-Tetraazatri(3.3.1.1(3,7))decane	0.0051	0.052
10203-30-2	3-Dodecanol	0.0010	0.015
10264-17-2	N-Hexylbutanamide	0.00005	0.1
103-23-1	bis(2-Ethylhexyl) hexandioate	0.0039	0.15
10374-14-8	2-Ethylcyclobutanone	0.0050	0.067
104-50-7	5-Butyldihydro-2(3H)-furanone	0.00087	5
104-61-0	5-Pentyldihydro-2(3H)-furanone	0.0025	0.5
104-67-6	5-Heptyldihydro-2(3H)-furanone	0.00069	15
104-76-7	2-Ethyl-1-hexanol	0.49	5
10486-19-8	Tridecanal	0.00023	0.5
104-90-5	5-Ethyl-2-methylpyridine	0.0026	0.02
105-21-5	5-Propyldihydro-2(3H)-furanone	0.0019	5
105-42-0	4-Methyl-2-hexanone	**1.1**	0.05
105-66-8	Propyl butanoate	0.042	15
10599-75-4	N-(Pentylidene)methanamine	0.022	0.05
10599-77-6	N-Pentylidene-1-butanamine	0.00063	0.01
1066-40-6	Trimethylsilanol	0.056	5
106-72-9	2,6-Dimethylhept-5-enal	0.067	25
1072-44-2	N-Methylaziridine	**0.065**	0.02
107-29-9	Ethanal oxime	Not Detected	0.1
1073-11-6	5-Ethenyl-5-methyldihydro-2(3H)-furanone	0.00044	0.5
107-51-7	Octamethyltrisiloxane	0.0068	3
107-75-5	7-Hydroxy-3,7-dimethyloctanal	0.00013	0.5
107-89-1	3-Hydroxybutanal	0.019	0.2
107-92-6	Butanoic acid	0.85	1
108-29-2	5-Methyldihydro-2(3H)-furanone	0.0098	75
108-30-5	Dihydro-2,5-furandione	0.0020	0.0025
1083-56-3	bis-1,1'-(1,4-Butanediyl)benzene	0.0014	1
108-47-4	2,4-Dimethylpyridine	**0.10**	0.02
108-48-5	2,6-Dimethylpyridine	0.0025	0.02
109-08-0	Methylpyrazine	0.0055	1
109-21-7	Butyl butanoate	0.40	1.5
109-69-3	1-Chlorobutane	0.15	0.75
109-75-1	3-Butenenitrile	**0.021**	0.02
109-93-3	Divinyl ether	0.031	2
109-95-5	Ethyl nitrite	Not Detected	0.2
109-97-7	1H-Pyrrole	0.011	0.03
110-00-9	Furan	**3.2**	0.01
110-13-4	2,5-Hexandione	0.0015	0.005
110-27-0	1-Methylethyl tetradecanoate	**0.17**	0.0035
110-36-1	Butyl tetradecanoate	**0.20**	0.0035
110-41-8	2-Methylundecanal	0.0048	0.5
110-59-8	Pentanenitrile	**1.1**	0.08
110-71-4	1,2-Dimethoxyethane	0.0025	100
110-74-7	Propyl formate	0.054	1

Table A.16. (contd)

CAS or TWINS Number	Chemical	Max. Conc. (ppm)	Screening Value (ppm)
110-93-0	6-Methyl-5-hepten-2-one	0.0012	0.15
111-06-8	Butyl hexadecanoate	0.00019	0.0035
111-13-7	2-Octanone	0.32	0.5
1112-39-6	Dimethoxydimethylsilane	0.011	5
111-27-3	1-Hexanol	0.073	1
1115-11-3	2-Methylbut-2-enal	**0.013**	0.003
111-70-6	1-Heptanol	0.40	0.5
111-71-7	Heptanal	0.12	0.5
1117-59-5	Hexyl pentanoate	0.0021	1.5
1120-06-5	2-Decanol	0.00068	0.015
1120-07-6	Nonanamide	0.0011	5
1120-64-5	2-Methyl-4,5-dihydrooxazole	0.016	0.5
1121-05-7	2,3-Dimethyl-2-cyclopenten-1-one	0.0013	0.05
1121-07-9	1-Methyl-2,5-pyrrolidinedione	0.0055	10
112-12-9	2-Undecanone	0.37	0.5
1121-33-1	2,4-Dimethylcyclopentanone	0.0052	0.2
112-30-1	1-Decanol	0.0011	0.15
112-31-2	Decanal	0.042	0.5
1123-28-0	1-Hydroxycyclohexanecarboxylic acid	0.018	0.3
112-42-5	1-Undecanol	0.00069	0.015
112-44-7	Undecanal	0.00053	0.5
112-53-8	1-Dodecanol	0.00096	0.015
112-54-9	Dodecanal	0.00067	0.5
112-72-1	1-Tetradecanol	0.0010	0.015
112-80-1	Z-Octadec-9-enoic acid	0.0055	1
112-88-9	1-Octadecene	0.00018	1
112-92-5	1-Octadecanol	**0.96**	0.015
112-95-8	Eicosane	0.016	2
1184-60-7	2-Fluoropropene	**0.53**	0.01
1191-95-3	Cyclobutanone	0.048	0.067
1191-99-7	2,3-Dihydrofuran	0.025	0.5
1192-33-2	3,3-Dimethylcyclobutanone	0.0011	0.067
1192-51-4	3-Methyl-2,4(3H,5H)-furandione	**0.0035**	0.0025
1196-92-5	4-Hydroxy-3-methoxybenzylmethanamine	0.0031	0.05
121-00-6	(1,1-Dimethylethyl)-4-methoxyphenol	0.00050	0.05
123-05-7	2-Ethylhexanal	0.033	0.5
123-08-0	4-Hydroxybenzaldehyde	0.0013	0.0046
123-15-9	2-Methylpentanal	0.051	0.50
123-25-1	Diethyl butanedioate	0.67	1.5
123-32-0	2,5-Dimethylpyrazine	0.00038	1
123-39-7	N-Methylformamide	Not Detected	0.4
123-56-8	2,5-Pyrrolidinedione	0.0025	10
123-79-5	Dioctyl hexandioate	0.099	0.15
123-95-5	Butyl octadecanoate	0.0019	0.0035
123-96-6	2-Octanol	0.070	0.5
124-12-9	Octanenitrile	**0.49**	0.08
124-13-0	Octanal	0.46	0.5
124-19-6	Nonanal	1.0	5
124-28-7	N,N-Dimethyl-1-octadecanamine	0.00030	0.1
13040-03-4	4,6,6-trimethyl-(1a,2b,5a)-bicyclo[3.1.1]hept-3-en-2-ol	0.00088	0.5
13287-23-5	8-Methylheptadecane	0.00018	2
13287-24-6	9-Methylnonadecane	0.00094	2
13475-75-7	8-Hexylpentadecane	0.0054	2
136-77-6	4-Hexyl-1,3-benzenediol	0.00063	0.2
137-32-6	2-Methyl-1-butanol	0.041	1

Table A.16. (contd)

CAS or TWINS Number	Chemical	Max. Conc. (ppm)	Screening Value (ppm)
13861-97-7	4,4-Dimethyldihydro-2(3H)-furanone	0.0012	0.5
13925-00-3	Ethylpyrazine	0.0065	0.1
14128-61-1	5-Methyl-5-phenyl-2-hexanone	0.0072	0.5
14129-48-7	4-Octen-3-one	0.0036	0.15
141-62-8	Decamethyltetrasiloxane	0.0027	3
142-30-3	2,5-Dimethyl-3-hexyne-2,5-diol	0.00036	0.1
142-60-9	Octyl propionate	0.0036	1.5
142-62-1	Hexanoic acid	0.00077	1
142-78-9	N-(2-Hydroxyethyl)dodecanamide	0.00072	5
142-91-6	1-Methylethyl hexadecanoate	**0.033**	0.0035
142-96-1	Dibutyl ether	0.39	1
143-07-7	Dodecanoic acid	0.034	1
143-08-8	1-Nonanol	0.0037	0.07
143-28-2	Z-9-Octadecen-1-ol	0.00042	1
14476-37-0	4-Undecanone	0.011	0.5
1454-84-8	1-Nonadecanol	0.00071	0.015
1454-85-9	1-Heptadecanol	0.0020	0.015
1462-84-6	2,3,6-Trimethylpyridine	0.00012	0.02
1467-79-4	Dimethylcyanamide	0.042	8
1482-15-1	3,4-Dimethyl-1-pentyn-3-ol	0.00054	1
1506-02-1	1-(5,6,7,8-Tetrahydro-3,5,5,6,8,8-hexamethyl-2-naphthenyl)ethanone	0.00009	0.1
151-18-8	3-Cyanopropanamine	0.00075	0.06
1534-26-5	3-Tridecanone	**0.61**	0.5
1534-27-6	3-Dodecanone	**1.1**	0.5
1560-88-9	2-Methyloctadecane	0.076	2
1565-81-7	3-Decanol	0.0026	0.015
1568-20-3	5-Methyl-4,5-dihydro-1H-pyrazole	0.018	0.02
1569-50-2	3-Penten-2-ol	0.0016	0.02
15726-15-5	3-Methyl-4-heptanone	0.0035	0.5
15877-57-3	3-Methylpentanal	0.042	0.17
15932-80-6	5-Methyl-2-(1-methylethylidene)cyclohexanone	0.043	0.2
1604-34-8	6,10-Dimethyl-2-undecanone	0.040	0.5
1615-70-9	2,4-Pentadienenitrile	**0.041**	0.02
1626-09-1	2,7-Octanedione	0.0070	0.05
1647-11-6	2-Methylene butanenitrile	**0.043**	0.02
16519-68-9	2,6-Dimethylcyclohexanone	0.00058	0.2
1653-30-1	2-Undecanol	0.00046	0.015
1653-31-2	2-Tridecanol	0.00056	0.015
16624-06-9	a,a-Dimethylcyclooctanemethanol	0.0023	0.015
1669-44-9	3-Octen-2-one	0.047	0.15
16778-26-0	3a,4,5,6-Tetrahydro-3a,6,6-trimethylbenzofuranone	0.090	0.5
1679-08-9	2,2-Dimethyl-1-propanethiol	0.066	7.3
1703-52-2	2-Ethyl-5-methylfuran	**0.010**	0.01
1708-29-8	2,5-Dihydrofuran	**1.8**	0.5
1712-64-7	1-Methylethyl nitrate	0.091	1
1713-33-3	1-Methyl-7-oxabicyclo[4.1.0]heptane	0.0021	0.05
17351-34-7	Pentadec-14-enoic acid	0.0039	1
17429-02-6	4-Hydroxy-4-methylcyclohexanone	0.00035	0.2
1757-42-2	3-Methylcyclopentanone	0.022	0.2
1759-53-1	Cyclopropanecarboxylic acid	0.054	0.1
17622-46-7	4-Ethyl-3,4-dimethyl-2-cyclohexen-1-one	0.00048	0.02
1779-19-7	1,3,6-Trioxocane	0.0016	0.2
17851-53-5	Butyl 2-methylpropyl phthalate	0.00085	0.0055
18344-37-1	2,6,10,14-Tetramethylheptadecane	0.0035	2
1838-59-1	2-Propenyl formate	**1.1**	1

Table A.16. (contd)

CAS or TWINS Number	Chemical	Max. Conc. (ppm)	Screening Value (ppm)
1840-42-2	Trinitrofluoromethane	0.015	10
18433-98-2	2,5-Dimethyl-3-(3-methylbutyl)pyrazine	0.0013	0.02
18435-45-5	1-Nonadecene	0.00008	1
18521-07-8	Z-2-Methyl-3-octen-2-ol	0.058	1
18829-55-5	E-Hept-2-enal	0.0016	0.003
18829-56-6	E-Non-2-enal	0.0029	0.003
1888-57-9	2,5-Dimethyl-3-hexanone	0.0057	0.5
18936-17-9	2-Methylbutanenitrile	0.040	0.08
19269-28-4	3-Methylhexanal	0.14	1
1927-69-1	Tetrahydro-2-(1,1-Dimethylethoxy)-2H-pyran	0.023	0.19
1932-92-9	2-Propyn-1-yl propanioate	0.0012	1.5
1937-62-8	Methyl E-9-octadecenoate	0.00064	0.0035
19549-80-5	4,6-Dimethyl-2-heptanone	0.00096	0.5
19550-03-9	2,3-Dimethyl-2-hexanol	0.00012	0.5
19550-46-0	1,3-Dimethylcyclopentanol	0.025	0.5
19550-73-3	trans-3,4-Dimethylcyclopentanone	0.00012	0.2
1975-78-6	Decanenitrile	**0.16**	0.08
19780-10-0	5-Dodecanone	0.024	0.5
19780-59-7	3-Ethyl-2-methyl-2-heptanol	0.00097	0.5
19780-63-3	3-Ethyl-2-methyl-2-pentanol	0.00017	0.25
19781-07-8	2,7-Dimethyl-2,7-octanediol	0.0027	0.5
19781-27-2	6-Ethyl-3-octanol	0.0013	0.5
20192-66-9	trans-Hexahydro-1,3-benzodioxol-2-one	0.00037	0.02
2040-07-5	1-(2,4,5-Trimethylphenyl)ethanone	0.0023	0.1
20474-93-5	2-Propenyl 2-butenoate	**0.29**	0.15
2050-78-4	Decyl nitrate	0.00095	0.25
20633-11-8	Hexyl nitrate	0.10	0.25
20633-12-9	Heptyl nitrate	0.10	0.25
20633-13-0	Nonyl nitrate	0.00017	0.25
20691-89-8	1-Methyl-4-piperidinemethanol	0.0075	0.01
20698-91-3	Methyl α-hydroxybenzeneacetate	0.0011	0.0035
20743-95-7	1-Butoxy-4-methoxybenzene	0.00050	0.01
20754-04-5	3-Methyl-4-octanone	0.0029	0.5
2091-29-4	Hexadec-9-enoic acid	0.33	1
20959-33-5	7-Methylheptadecane	0.044	2
21078-65-9	2-Ethyl-1-decanol	0.00012	0.015
21164-95-4	7,9-Dimethylhexadecane	0.0011	2
2136-70-1	2-Tetradecyloxyethanol	0.18	0.2
215229-01-9	Ethyl peroxynitrite	Not Detected	0.01
22026-12-6	6-Tridecanone	0.099	0.5
2216-87-7	3-Undecanone	0.11	0.5
22319-25-1	4-Methyl-3-hepten-2-one	0.0071	0.15
22319-29-5	5-Ethyl-2,4-dimethyl-4-hepten-3-one	0.031	0.15
22431-09-0	N-(1-Methylbutylidene)methanamine	**0.13**	0.05
2243-27-8	Nonanonitrile	**0.16**	0.08
2244-07-7	Undecanenitrile	0.00029	0.08
2345-27-9	2-Tetradecanone	0.011	0.5
23462-75-1	Dihydro-2H-pyran-3(4H)-one	0.0010	1
2371-19-9	3-Methyl-2-heptanone	0.0086	0.5
2407-94-5	1,1'-Dioxybiscyclohexanol	0.00019	0.5
2408-37-9	2,2,6-Trimethylcyclohexanone	0.030	0.2
2425-77-6	2-Hexyl-1-decanol	0.025	0.2
24405-16-1	Tetrahydro-5,6-dimethyl-2H-pyran-2-one	0.21	1
2456-28-2	Didecyl ether	0.073	1
2490-48-4	2-Methyl-1-hexadecanol	0.00039	0.0015

Table A.16. (contd)

CAS or TWINS Number	Chemical	Max. Conc. (ppm)	Screening Value (ppm)
25013-16-5	2-(1,1-Dimethylethyl)-4-methoxyphenol	0.00037	0.05
2508-29-4	5-Hydroxy-1-pentanamine	0.00065	0.05
2548-87-0	E-Oct-2-enal	0.0016	0.003
2549-67-9	2-Ethylaziridine	**0.056**	0.02
25564-22-1	2-Pentyl-2-cyclopenten-1-one	0.040	0.05
2610-95-9	Tetrahydro-6,6-dimethyl-2H-pyran-2-one	0.00052	1
26215-90-7	4-Tridecanone	0.019	0.5
26248-42-0	Tridecanol	0.0011	0.0015
2639-63-6	Hexyl butanoate	0.00013	1.5
26465-81-6	2,3-Dihydro-3,3-dimethyl-1H-inden-1-one	0.00042	0.01
26496-20-8	4-Tetradecanone	0.0014	0.5
26537-19-9	Methyl 4-(1,1-dimethylethyl)benzoate	0.00052	0.00055
27392-16-1	trans-2-(1,1-Dimethylethyl)-cyclohexanecarboxylic acid	0.00024	0.00066
27675-36-1	Z-1-Nitropropene	0.0021	0.25
28019-94-5	4,5-Dimethyl-4,5-dihydro-1H-pyrazole	0.0055	0.02
28290-01-9	2,3,3-Trimethylcyclobutanone	0.0021	0.067
28473-21-4	Nonanol	0.0032	0.07
2865-82-9	5-Ethyldihydro-5-methyl-2(3H)-furanone	0.0014	0.5
288-16-4	Isothiazole	0.00079	0.01
288-47-1	Thiazole	0.0024	0.1
288-88-0	1H-1,2,4-Triazole	0.0087	1
289-95-2	Pyrimidine	0.029	3
29006-00-6	6-Methoxy-3-hexanone	0.00011	2
2902-96-7	2-Nitro-1-propanol	**0.43**	0.1
290-37-9	Pyrazine	0.12	2
2919-23-5	Cyclobutanol	0.0055	0.5
2922-51-2	2-Heptadecanone	0.00009	0.5
29354-98-1	Hexadecanol	0.00009	0.0015
29366-35-6	11-Methyl-4-decanone	0.0029	0.5
298-12-4	Glyoxylic acid	Not Detected	12
29887-79-4	trans-1,3-Dimethoxycycloheptane	0.00028	0.2
3031-73-0	Methyl hydroperoxide	Not Detected	0.01
3031-74-1	Ethyl hydroperoxide	Not Detected	0.01
3054-92-0	2,3,4-Trimethyl-3-pentanol	0.0017	0.25
30692-16-1	5-Tridecanone	0.0034	0.5
30951-17-8	Decahydro-4a-methyl-8-methylene-2-(1-methylethyl)-1-naphthalenol	0.00071	0.5
31681-26-2	alpha-Propyl-2-furanacetaldehyde	**0.030**	0.02
32064-72-5	2-Nonen-4-one	0.010	0.15
33083-83-9	5-Undecanone	0.016	0.5
334-48-5	Decanoic acid	0.00039	1
33933-82-3	5,9-Dimethyl-2-decanone	0.0029	0.5
34314-82-4	3-(1,1-Dimethylethyl)-2,3-dihydrofuran	0.00053	0.5
34379-54-9	4-(1-Methylpropyl)-2,3-dihydrofuran	0.00098	0.5
3438-46-8	4-Methylpyrimidine	0.0091	0.3
34386-42-0	4-(1,1-Dimethylethyl)-a-methylbenzenemethanol	0.0031	0.01
3457-90-7	1,3-Propanediol, dinitrate	**0.018**	0.0005
3457-91-8	1,4-Butanediol, dinitrate	**0.26**	0.0005
3457-92-9	1,5-Pentanediol, dinitrate	**0.0032**	0.0005
35194-30-0	9-Decen-2-one	0.00048	0.15
35468-97-4	1-Hepten-1-yl acetate	0.0034	1.5
35996-97-5	Butyl pentadecanoate	0.00062	0.0035
3622-84-2	N-Butylbenzenesulfonamide	**0.16**	0.015
3664-60-6	7-Octen-2-one	0.0012	0.15
36653-82-4	1-Hexadecanol	**1.1**	0.015
3682-42-6	Methyl 2-oxo-3-methylpentanoate	0.0036	1.5

Table A.16. (contd)

CAS or TWINS Number	Chemical	Max. Conc. (ppm)	Screening Value (ppm)
3760-54-1	1-Pyrrolidinecarboxylaldehyde	0.00014	0.1
3760-63-2	4-(Dimethylamino)-1-phenyl-1-butanone	0.0019	0.01
3761-94-2	1-Methylcycloheptanol	0.00017	0.5
3777-69-3	2-Pentylfuran	0.0025	0.01
3777-71-7	2-Heptylfuran	0.045	0.1
3789-85-3	Trimethylsilyl ester of 2-(trimethylsilyloxy)benzoic acid	0.017	0.25
3796-70-1	E-6,10-Dimethyl-5,9-undecadien-2-one	0.00008	0.15
38447-22-2	bis(1-Methylpropyl) hexanedioate	0.00017	0.15
3879-26-3	Z-6,10-Dimethyl-5,9-undecadien-2-one	0.00077	0.15
3892-00-0	2,6,10-Trimethylpentadecane	0.0083	2
3913-02-8	2-Butyl-1-octanol	0.042	0.5
3913-81-3	E-Dec-2-enal	0.00062	0.003
39161-19-8	3-Penten-1-ol	0.0069	0.02
39168-02-0	trans-2,4-Dimethyltetrahydrofuran	0.0032	0.5
3944-36-3	1-(1-Methylethoxy)-2-propanol	0.0063	0.2
39515-51-0	3-Phenoxybenzaldehyde	0.00023	0.0023
39899-08-6	3-Methyl-3-hepten-2-one	0.026	0.15
40649-36-3	4-Propylcyclohexanone	0.034	0.2
40702-26-9	1,3,4-Trimethylcyclohex-3-en-1-carboxaldehyde	0.00074	0.003
4088-60-2	Z-2-Buten-1-ol	0.037	0.07
41239-48-9	2,5-Diethyltetrahydrofuran	0.019	0.5
41744-75-6	16-Methyl-1-heptadecanol	0.00033	0.0015
4176-04-9	4,7,7-Trimethylbicyclo[4.1.0]heptan-3-one	**0.086**	0.02
4179-38-8	2-Octylfuran	0.00081	0.01
420-05-3	Cyanic acid	Not Detected	0.047
420-56-4	Fluorotrimethylsilane	0.00049	0.05
4229-91-8	2-Propylfuran	**0.60**	0.01
42565-49-1	2,2,6,6-Tetramethyl-10-undecen-4-one	0.0014	0.15
42604-04-6	Methoxycycloheptane	0.019	0.2
4272-06-4	4-Undecanol	0.00030	0.015
42786-06-1	3-Amino-4-ethyl-4H-1,2,4-triazole	0.0019	1
42829-59-4	Methyl peroxynitrate	Not Detected	0.03
4312-99-6	1-Octen-3-one	0.0060	0.15
4337-65-9	2-Ethylhexyl hexandioate	0.0026	0.15
4457-62-9	2,5-Dipropyltetrahydrofuran	0.00097	0.5
4485-09-0	4-Nonanone	0.12	0.5
4562-27-0	4(1H)-Pyrimidinone	0.0016	0.1
4573-09-5	2,2,5-Trimethylcyclopentanone	0.0026	0.2
460-13-9	1-Fluoropropane	0.057	0.75
4631-98-5	4-(1,1,3,3-Tetramethylbutyl)cyclohexanol	0.00045	0.5
463-58-1	Carbonyl sulfide	0.026	1
470-65-5	4-Methyl-1-(1-methylethyl)cyclohexanol	0.00018	0.5
4786-20-3	2-Butenenitrile	0.0057	0.02
4799-62-6	5-Methoxy-1-pentanol	0.0021	1
4826-62-4	Dodec-2-enal	0.00049	0.003
484678-32-2	Methyl peroxynitrite	Not Detected	0.01
486-25-9	9H-Fluoen-9-one	0.0021	0.01
4911-70-0	2,3-Dimethyl-2-pentanol	0.0012	0.25
502-56-7	5-Nonanone	0.0024	0.005
502-69-2	6,10,14-Trimethyl-2-pentadecanone	0.00047	0.5
503-30-0	Trimethylene oxide	0.56	2.5
5057-99-8	trans-1,2-Cyclopentanediol	0.0018	0.1
50639-02-6	2-Methyl-5-undecanone	0.20	0.5
507-55-1	1,3-Dichloro-1,1,2,2,3-pentafluoropropane	1.0	1.667
5115-98-0	N-Methyl-3-piperidinecarboxamide	0.0015	1

Table A.16. (contd)

CAS or TWINS Number	Chemical	Max. Conc. (ppm)	Screening Value (ppm)
51411-24-6	3,7,11-Trimethyl-6,10-dodecadien-1-ol	0.26	1
5145-01-7	3,5-Dimethyldihydro-2(3H)-furanone	0.14	0.5
51595-87-0	2-(2-Methyl-6-oxoheptyl)furan	0.00052	0.01
5166-53-0	5-Methyl-3-hexen-2-one	0.0034	0.15
517-25-9	Trinitromethane	Not Detected	0.2
51756-19-5	2-Methyl-1-nonen-3-one	0.00087	0.15
51953-17-4	4(3H)-Pyrimidinone	0.0051	0.1
5204-80-8	2-Ethylpent-4-enal	0.014	5
5205-34-5	5-Decanol	0.0035	0.015
52588-78-0	6,6-Dimethyl-3,4-undecadien-2,10-dione	0.00022	0.015
53229-39-3	(1-Methylbutyl)oxirane	0.00046	0.02
53398-83-7	E-2-Hexenyl butanoate	0.0053	1.5
534-22-5	2-Methylfuran	**1.0**	0.01
53535-33-4	Heptanol	0.059	0.5
53833-32-2	2-n-Propyl-4,5-dimethyloxazole	0.0075	0.5
53907-75-8	2-Methyl-2-pentyloxirane	0.0028	0.02
54004-41-0	4-Methyl-2-propyl-1-pentanol	0.0055	0.25
541-05-9	Hexamethylcyclotrisiloxane	0.63	4.4
541-35-5	Butanamide	0.020	0.1
541-73-1	1,3-Dichlorobenzene	0.010	0.25
542-44-9	2,3-Dihydroxypropyl hexadecanoate	0.00027	0.0035
542-54-1	4-Methylpentanenitrile	0.024	0.08
542-55-2	2-Methylpropyl formate	0.066	1
542-56-3	2-Methyl-1-propyl nitrite	0.025	0.1
543-29-3	2-Methylpropyl nitrate	0.070	0.25
543-49-7	2-Heptanol	0.052	0.5
543-87-3	3-Methyl-1-butyl nitrate	0.15	0.25
544-16-1	Butyl nitrite	**0.49**	0.4
544-63-8	Tetradecanoic acid	0.39	1
5454-28-4	Butyl heptanoate	0.0011	0.15
54658-01-4	3-Methoxyhexane	0.045	0.05
54774-28-6	trans-5-Methyltetrahydrofuranmethanol	0.00065	0.02
54833-48-6	2,6,10,15-Tetramethylheptadecane	0.00060	2
54845-28-2	(E,E)-2-Hexenyl 2-hexenoate	0.035	0.15
5500-21-0	Cyclopropanenitrile	0.0073	0.06
55282-34-3	1,3,5,-Trimethyl-2-octadecylcyclohexane	0.0086	1
55373-86-9	7-Hexyldocosane	0.0035	2
55429-85-1	N-[Perfluorophenyl]-beta,4-bis(trimethylsilyloxy)benzeneethanamine	0.0039	1
556-67-2	Octamethylcyclotetrasiloxane	0.41	3
55956-20-2	5-Methyl-3-(2-propenyl)-2-oxazolidinone	0.011	0.5
56052-85-8	E-5-Pentyloxy-2-pentene	0.0034	1
56052-94-9	cis-2-Ethyl-3-propyloxirane	**0.030**	0.02
56-40-6	Glycine	Not Detected	100
56554-96-2	Octadec-2-enal	0.0020	0.003
565-61-7	3-Methyl-2-pentanone	0.036	0.5
565-67-3	2-Methyl-3-pentanol	0.073	0.25
565-68-4	4-Methyl-1-pentyn-3-ol	0.0098	1
565-69-5	2-Methyl-3-pentanone	0.013	0.5
565-80-0	2,4-Dimethyl-3-pentanone	0.061	0.5
5675-51-4	1,12-Dodecanediol	0.00011	0.0015
57-10-3	Hexadecanoic acid	0.37	1
57-11-4	Octadecanoic acid	0.00032	1
5715-25-3	4,5-Dimethyl-2-cyclohexen-1-one	0.0044	0.02
5746-58-7	12-Methyltetradecanoic acid	0.00088	1
5756-43-4	1-Ethoxyhexane	0.019	0.05

Table A.16. (contd)

CAS or TWINS Number	Chemical	Max. Conc. (ppm)	Screening Value (ppm)
57706-88-4	3,7-Dimethyl-3-octanol	0.0012	0.5
5775-96-2	4,5-Dihydro-1,5-dimethyl-1H-pyrazole	0.0071	0.2
578-54-1	2-Ethylbenzenamine	0.0015	0.005
583-58-4	3,4-Dimethylpyridine	0.0015	0.02
58467-28-0	3-Ethyl-3-hydroxy-2,5-pyrrolidinedione	0.0011	10
5857-36-3	2,2,4-Trimethyl-3-pentanone	0.012	0.5
585-74-0	1-(3-Methylphenyl)ethanone	0.00033	0.1
589-38-8	3-Hexanone	**6.3**	2
589-63-9	4-Octanone	0.47	0.5
589-82-2	3-Heptanol	0.065	0.5
589-93-5	2,5-Dimethylpyridine	0.019	0.02
590-01-2	Butyl propionate	0.20	1.5
590-36-3	2-Methyl-2-pentanol	0.051	0.25
590-50-1	4,4-Dimethyl-2-pentanone	0.11	0.5
590-86-3	3-Methylbutanal	0.085	0.5
5910-87-2	E,E-Nona-2,4-dienal	0.00087	0.003
5910-89-4	2,3-Dimethylpyrazine	0.0089	0.5
591-22-0	3,5-Dimethylpyridine	0.0021	0.02
591-23-1	3-Methylcyclohexanol	0.00059	0.5
591-24-2	3-Methylcyclohexanone	0.029	0.2
591-87-7	2-Propenyl acetate	1.0	5
592-84-7	Butyl formate	0.72	1
593-08-8	2-Tridecanone	0.24	0.5
593-45-3	Octadecane	0.0065	2
594-70-7	2-Nitro-2-methylpropane	**0.23**	0.1
59681-06-0	2,6,10,19,23-Pentamethyl-2,6,10,14,18,22-tetracoshexaene	0.060	5
59681-06-0	2,6,10,14,18,22-Tetracosahexaene, 2,6,10,19,23-pentamethyl-, (all-E)-	0.060	5
598-32-3	3-Buten-2-ol	0.026	5
598-58-3	Methyl nitrate	0.33	1.3
59-89-2	N-Nitrosomorpholine	**0.0097**	0.005
59983-39-0	2-(Methoxymethyl)-1-pyrrolidinamine	0.00031	0.1
600-14-6	2,3-Pentadione	0.016	0.2
600-24-8	2-Nitrobutane	0.0012	0.1
600-40-8	1,1-Dinitroethane	Not Detected	1
6032-29-7	2-Pentanol	0.14	5
60-35-5	Acetamide	0.0032	0.01
6064-27-3	6-Dodecanone	0.090	0.5
608-25-3	2-Methyl-1,3-benzenediol	0.00099	10
61142-47-0	2-Methoxy-2-pentene	0.00056	0.5
6137-06-0	4-Methyl-2-heptanone	0.017	0.5
6137-12-8	4-Ethyl-3-hexanone	0.00059	0.5
6137-26-4	4-Dodecanone	0.026	0.5
613-93-4	N-Methylbenzamide	0.00033	0.005
616-45-5	2-Pyrrolidinone	**0.25**	0.1
617-29-8	2-Methyl-3-hexanol	0.018	0.06
6175-49-1	2-Dodecanone	0.018	0.5
617-94-7	Phenyl-a,a-dimethylmethanol	**2.2**	0.1
623-37-0	3-Hexanol	0.0081	0.06
623-56-3	5-Methyl-3-hexanone	0.0017	0.5
623-87-0	1,2,3-Propanetriol, 1,3-dinitrate	**0.010**	0.0005
624-16-8	4-Decanone	0.0026	0.5
624-42-0	6-Methyl-3-heptanone	0.0052	0.25
624-43-1	1,2,3-Propanetriol, 1-nitrate	**0.026**	0.0005
624-91-9	Methyl nitrite	**0.32**	0.2

Table A.16. (contd)

CAS or TWINS Number	Chemical	Max. Conc. (ppm)	Screening Value (ppm)
624-95-3	3,3-Dimethyl-1-butanol	0.018	1
625-25-2	2-Methyl-2-heptanol	0.00069	0.5
625-58-1	Ethyl nitrate	0.40	1.3
625-74-1	2-Methyl-1-nitropropane	0.0020	0.1
625-76-3	Dinitromethane	Not Detected	0.2
625-84-3	2,5-Dimethyl-1H-pyrrole	0.0027	0.01
625-86-5	2,5-Dimethylfuran	0.0093	0.01
627-05-4	1-Nitrobutane	**0.39**	0.25
627-27-0	3-Buten-1-ol	**5.7**	0.07
627-59-8	5-Methyl-2-hexanol	0.00051	0.5
6281-96-5	N-(2-Methylpropyl)formamide	0.0058	0.1
628-28-4	1-Methoxybutane	**0.43**	0.05
628-44-4	2-Methyl-2-octanol	0.0056	0.5
628-61-5	2-Chlorooctane	0.00071	0.01
628-73-9	Hexanenitrile	**0.85**	0.08
628-80-8	1-Methoxypentane	0.0077	0.2
629-08-3	Heptanenitrile	**0.64**	0.08
629-23-2	3-Tetradecanone	0.14	0.5
6295-06-3	Butyl glyoxalate	0.00025	1.5
629-54-9	Hexadecanamide	0.00026	5
629-60-7	Tridecanenitrile	0.052	0.08
629-70-9	1-Hexadecyl acetate	0.0043	1.5
629-76-5	1-Pentadecanol	0.0021	0.015
629-80-1	Hexadecanal	0.00044	0.5
629-89-0	1-Octadecyne	0.00018	10
629-92-5	Nonadecane	0.00025	2
629-94-7	Heneicosane	0.00098	2
630-01-3	Hexacosane	0.018	2
630-02-4	Octacosane	0.054	2
630-18-2	2,2-Dimethylpropanenitrile	0.021	0.08
630-19-3	2,2-Dimethylpropanal	0.020	0.25
637-88-7	1,4-Cyclohexanedione	0.0034	0.067
638-36-8	2,6,10,14-Tetramethylhexadecane	0.025	2
64160-40-3	Ethyl peroxynitrate	Not Detected	0.03
6418-44-6	3-Methylheptadecane	0.0044	2
645-56-7	4-Propylphenol	0.00051	0.05
645-62-5	2-Ethylhex-2-enal	**0.028**	0.003
66-25-1	Hexanal	1.3	5
6711-26-8	2,5-Dimethyl-2-(1-methylethenyl)cyclohexanone	0.00040	0.02
6728-26-3	E-Hex-2-enal	0.00030	0.003
6728-31-0	Z-Hept-4-enal	0.0020	5
6789-80-6	Z-Hex-3-enal	0.0047	5
6836-38-0	6-Dodecanol	0.0017	0.015
68443-63-0	Butyl 2-ethylhexanoate	0.0012	0.15
68820-35-9	E-Undec-4-enal	0.0024	5
6898-69-7	N-(Butylidene)methanamine	0.029	0.05
6898-74-4	N-Ethylidene-1-butanamine	0.0079	0.01
693-54-9	2-Decanone	0.086	0.5
693-98-1	2-Methyl-1H-imidazole	0.00043	0.1
694-05-3	1,2,3,6-Tetrahydropyridine	**0.093**	0.05
695-06-7	5-Ethyldihydro-2(3H)-furanone	0.017	5
69687-91-8	4-Methylphenyl 2-hexenoate	0.0014	0.15
69770-96-3	2-Methyl-4-(2-methylpropyl)cyclopentanone	0.068	0.2
699-22-9	1-Pentyl-1H-pyrrole	0.016	0.1
705-15-7	1-(2-Hydroxy-5-methoxyphenyl)ethanone	0.013	0.1

Table A.16. (contd)

CAS or TWINS Number	Chemical	Max. Conc. (ppm)	Screening Value (ppm)
706-14-9	5-Hexyldihydro-2(3H)-furanone	0.00079	5
7112-02-9	N-(2-Hydroxyethyl)octanamide	0.0034	0.5
71-41-0	1-Pentanol	0.12	0.2
717-21-5	2-(3-Oxo-3-phenylprop-1-enyl)furan	0.00058	0.01
719-22-2	2,6-bis(1,1-Dimethylethyl)-2,5-cyclohexdiene-1,4-dione	0.0029	0.01
7225-64-1	9-Octylheptadecane	0.017	2
7250-80-8	N-Hexylbenzenesulfonamide	0.00043	0.0015
7379-12-6	2-Methyl-3-hexanone	0.064	0.5
74367-34-3	3-Hydroxy-2,4,4-trimethylpentyl-2-methylpropanoate	0.00052	0.15
74381-40-1	1-(1,1-Dimethylethyl)-2-methyl-1,3-propanediyl 2-methylpropanoate	**0.45**	0.1
74646-36-9	1-Dodecyn-4-ol	0.0051	1
74646-37-0	1-Tridecyn-4-ol	0.00065	1
74685-30-6	E-5-Eicosene	0.054	1
74793-02-5	2,2-Bioxepane	0.045	0.05
75011-90-4	5-Propyl-4,5-dihydro-1H-pyrazole	0.0045	0.02
75-13-8	Isocyanic acid	Not Detected	0.13
75163-97-2	2,6-Dimethyloctadecane	0.00016	2
75-17-2	Methanal oxime	Not Detected	0.1
753-89-9	1-Chloro-2,2-dimethylpropane	0.0037	0.75
75-84-3	2,2-Dimethyl-1-propanol	0.036	0.5
75-85-4	2-Methyl-2-butanol	0.018	10
75-97-8	3,3-Dimethyl-2-butanone	0.034	2
76-09-5	2,3-Dimethyl-2,3-butanediol	0.0017	0.1
763-93-9	3-Hexen-2-one	0.011	0.15
766-15-4	4,4-Dimethyl-1,3-dioxane	0.0017	0.02
7683-64-9	2,6,10,15,19,23-Hexamethyl-2,6,10,14,18,22-tetracoshexaene	0.066	5
7726-08-1	N-(2-Hydroxyethyl)decanamide	0.00057	5
774-40-3	Ethyl α-hydroxybenzeneacetate	0.0017	0.0035
78-46-6	Dibutyl butylphosphonate	**0.070**	0.002
78-76-2	2-Bromobutane	**0.023**	0.01
78-85-3	2-Methylprop-2-enal	0.026	0.2
78-96-6	1-Amino-2-propanol	0.19	0.2
79-14-1	Glycolic acid	Not Detected	1.2
79-16-3	N-Methylacetamide	0.00037	0.1
79-31-2	2-Methylpropionic acid	0.010	1
80-39-7	N-Ethyl-N-methylbenzenesulfonamide	0.0014	0.0015
814-78-8	3-Methyl-3-buten-2-one	**0.021**	0.002
819-97-6	1-Methylpropyl butanoate	0.00016	1.5
820-29-1	5-Decanone	0.0061	0.5
821-41-0	5-Hexen-1-ol	0.016	0.02
821-55-6	2-Nonanone	**1.6**	0.5
83321-16-8	2,3,4-Trimethyl-3-cyclopenten-1-one	0.00081	0.15
84-64-0	Butyl cyclohexyl phthalate	0.0059	0.055
85-69-8	Butyl 2-ethylhexyl phthalate	0.00060	0.0055
865-40-7	Nitrosomethane	0.096	0.2
871-71-6	N-Butylformamide	0.013	0.1
873-94-9	3,3,5-Trimethylcyclohexanone	0.034	0.2
89-82-7	5-Methyl-2-(1-methylethenyl)cyclohexanone	**0.37**	0.2
91894-15-4	4-Methoxy-6-methyl-6,7-dihydro-4H-furo[3,2-c]pyran	0.078	1
922-63-4	2-Methylenebutanal	0.012	0.2
922-65-6	1,4-Pentadien-3-ol	0.0073	0.02
925-54-2	2-Methylhexanal	0.053	1
925-78-0	3-Nonanone	0.14	0.5
925-91-7	Nitrosoethane	Not Detected	0.2
926-42-1	2,2-Dimethyl-1-propyl nitrate	0.078	0.25

Table A.16. (contd)

CAS or TWINS Number	Chemical	Max. Conc. (ppm)	Screening Value (ppm)
928-45-0	Butyl nitrate	**0.36**	0.25
928-68-7	6-Methyl-2-heptanone	**2.1**	0.5
928-80-3	3-Decanone	0.0049	0.5
930-02-9	1-Ethenyloxyoctadecane	0.044	0.5
930-36-9	1-Methyl-1H-pyrazole	0.0018	0.02
93-55-0	1-Phenyl-1-propanone	0.047	0.1
948-65-2	2-Phenyl-1H-indole	0.00065	0.1
95-16-9	Benzothiazole	0.0099	1
96-17-3	2-Methylbutanal	0.021	0.5
96-41-3	Cyclopentanol	**1.9**	0.5
96-47-9	2-Methyltetrahydrofuran	0.039	0.5
96-48-0	Dihydro-2(3H)-furanone	0.91	75
97475-10-0	E,E-Dodeca-7,9-dienal	0.067	5
97-87-0	Butyl 2-methylpropionate	0.0040	1.5
97-95-0	2-Ethyl-1-butanol	0.012	1
98-54-4	4-(1,1-Dimethylethyl)phenol	0.0013	0.05
98-85-1	1-Phenylethanol	0.0047	0.01
ARUP0-9	Di-t-butyl-ethylphenol	0.00041	0.05
OHUES0-01	1-Heptadecanyl acetate	0.00008	1.5
UAD010-01	Decadienal	**0.015**	0.003
UAK018-01	C18-Alkane	0.0031	2
UAK020-01	C20-Alkane	0.012	2
UCA014-01	C14-Alkanoic acid	0.11	1
UCA016-01	C16-Alkanoic acid	**1.1**	1
UES010-01	C6 Ester of butanoic acid	0.00013	0.15
UES013-01	1-Ethylpropyl octanoate	0.00007	0.0035
UET005-01	C5-Ether	0.014	2
UHC000-05	C3-Pyridine	0.0015	0.05
UHC000-06	C4-2-Pyrrolidinone	0.00059	1
UHC000-07	C4-Piperidine	0.00069	0.01
UHC000-09	Methylpyridine	**0.52**	0.02
UHC000-10	C2-Pyrrolidine	0.29	0.4
UHC000-13	C2-Pyridine	**0.19**	0.05
UIN000-01	Sulfur oxides (SOx)	**0.37**	0.02
UKE006-01	C6-Alkanone	0.021	0.05
UKE006-02	C6-Alkenone	0.0021	0.15
UKE006-03	4-Hydroxy-4-methylpentanone	0.0034	0.05
UKE007-02	C7-Alkanone	0.071	0.5
UKE008-01	C8-Alkanone	**1.2**	0.5
UKE009-02	C9-Alkenone	0.13	0.15
UKE009-03	C9-Alkanone	1.1	0.5
UKE010-01	C10-Alkanone	0.027	0.5
UKE010-02	3-(2-Methyl-2-butyl)cyclopropanone	0.0016	0.067
UKE010-02	3-(2-Methyl-2-butyl)cyclopentanone	0.0016	0.067
UKE011-02	C11-Alkanone	0.013	0.5
UKE012-02	C12-Alkanone	0.41	0.5
UKE013-02	C13-Alkanone	**1.1**	0.5
UKE014-01	C14-Alkanone	0.050	0.5
UKE014-03	3-Cyclohexylidene-4-ethyl-2-hexanone	0.029	0.05
UKE015-01	4-Cyclohexylidene-3,3-diethyl-2-pentanone	0.017	0.15
UNA003-01	C3-Nitrate	0.019	0.25
UNI007-01	C7-Nitrile	0.011	0.08
UNI008-01	C8-Nitrile	0.018	0.08
UOH010-01	1-Cyclopentyl-2,2-dimethyl-1-propanol	0.017	0.5

Table A.16. (contd)

CAS or TWINS Number	Chemical	Max. Conc. (ppm)	Screening Value (ppm)
UPH000-01	Octylphenol	0.00011	0.05
UPHUSI-01	Nonylphenol	0.00010	0.05
USA000-02	C6-Benzenesulfonamide	0.00035	0.0015
USI000-05	Trimethylsilyl ester of methoxybenzoic acid	0.0015	0.25

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