

## **Appendix A**

### **Publicly Available Protocols for the ICE Test Method**

<b>A1</b>	<b>INVITTOX Protocol 80. The Chicken Enucleated Eye Test (CEET) – Method of Prinsen .....</b>	<b>A-3</b>
<b>A2</b>	<b>Table of ICE Protocols .....</b>	<b>A-19</b>

***[This Page Intentionally Left Blank]***

## **Appendix A1**

### **INVITTOX Protocol 80. The Chicken Enucleated Eye Test (CEET) – Method of Prinsen**

***[This Page Intentionally Left Blank]***

## CHICKEN ENUCLEATED EYE TEST (CEET)

The isolated eye of a chicken is exposed to the test compound and assessed for corneal swelling, corneal opacity and fluorescein retention in order to evaluate the eye irritation potential of the compound.

---

### Contact

**Dr. Menk Prinsen**

TNO-CIVO Institutes

POB 360

Utrechtsweg 48

3700 AJ ZEIST

Netherlands

Tel: +31 3404 44558

Fax: +31 3404 57224

### **NOTE**

*The protocol presents the standard operation procedure used in the Home Office UK/EEC Validation Study for Alternatives to the Draize Test. It should be noted that this protocol might need to be modified in light of experience gained in the study. Additional information added in the course of producing this **INVITTOX** protocol, e.g. this note, is presented in italics. In addition, Annex 3, the representative data presented in Table 1 and the list of bibliographical references were not part of the original study SOP. An English language version of the SOP for this test system, as used at TNO, is available on request from Dr. Prinsen.*

---

## Critical Assessment

This protocol was used in an international validation study on alternatives to the Draize eye irritation test for the classification and labelling of chemicals. In this project, nine promising non-animal alternative methods to the Draize Eye Test were selected to undergo final validation. Each of the nine methods was examined by four laboratories and about 60 compounds were tested. The goal of the project was to select those methods which could serve as a valid prescreen or complete replacement of the Draize Eye Test.

The Enucleated Eye Test (EET) with isolated eyes of rabbits has been recognized as a valuable alternative to the Draize eye irritation test, because it represents a test system nearest to the *in vivo* test, without the need to use live animals. However, it is preferable to use slaughterhouse waste tissue as a source of eyes for this procedure. Of the possible eye-donor species, such as the cow, the pig, or the chicken, the latter has been found to be the most suitable for the assessment of eye irritation potential of test materials.

In the Chicken Enucleated Eye Test (CEET), the test compound is applied in one single dose onto the corneas of isolated eyes, which are obtained from slaughterhouse animals after these have been killed. Three parameters are measured to disclose possible adverse eye effects, namely corneal thickness (expressed as corneal swelling), corneal opacity and fluorescein retention of damaged epithelial cells of the cornea. The measurement of corneal swelling in this assay guarantees a highly objective parameter, which enables the investigator to discriminate the damaging effects of test materials very precisely. In combination with the measurement of corneal opacity and fluorescein retention, though assessed by subjective observation, but being accurately measured by the use of a slit-lamp microscope, a reliable evaluation of the eye irritation potential of test materials can be achieved.

---

## Chemicals Tested

Liquid materials are applied with a micropipette in a standard dosing volume of 30  $\mu$ l. Pastes may be softened by means of a warm water bath (c. 70°C), collected with the micropipette and applied after cooling down to a lukewarm temperature. This procedure is also applicable when dealing with highly viscous liquids, if they cannot be handled properly at room temperature.

The procedure followed should be noted on the scoring form.

Solids, ground to a fine powder if necessary, are applied by powdering the entire surface of the cornea with a standard amount of 30 mg.

In addition, prior to or during testing, the hydrophobicity or hydrophilicity of liquid materials should be established. This can easily be done by putting some of the compound in a beaker with water and observing whether or not the compound mixes with the water.

---

## Procedure Details

### Principle

The test compound is applied onto the corneas of at least three eyes in one single dose. Prior to dosing, each test eye provides its own baseline values for the assessment of corneal effects. One untreated eye serves as a control of the experimental conditions. The reactions of the corneas are examined at regular intervals for up to four hours after treatment. Based on the mean

scores for corneal swelling, corneal opacity and fluorescein retention, an assessment of the eye irritation potential of the compound, ranging from non- to severely irritating, can be made.

### **Experimental design**

In the past, the Enucleated Eye Test has been performed in three of the four laboratories participating in the validation study with this method, using different types of equipment, such as the slit-lamp microscope. Different slit-lamp microscopes and depth measuring devices can give rise to a variation in the swelling ranges obtained. However, ranking of the compounds according to the swelling figures should be similar, regardless of the apparatus.

Since a variation in equipment and in the source of the chickens cannot be avoided, only general directions with respect to these items can be given in the protocol.

Chicken eyes are carefully dissected and placed in a superfusion apparatus using the following procedure:

First the eyelids are carefully removed without damaging the cornea, and a small drop of fluorescein sodium (0.5-2%) is applied to the corneal surface for a few seconds and subsequently rinsed off with isotonic saline at ambient temperature.

*N.B.. both 0.5% and 2% concentrations of fluorescein were used by laboratories in the EEC/Colipa study. A 2% concentration is recommended, and is available as Fluorescein sodium BP 2% w/v (Minims, Smith and Nephew Ltd., Romford, England). Usually a flush of 5 ml isotonic saline is sufficient to rinse away the fluorescein that has not been retained by the cornea, but a longer rinsing period may be used if required.*

Then, the head with the fluorescein-treated cornea is examined with a slit-lamp microscope (Slit-lamp 900 CN, Haag-Streit AG, Liebefeld-Bern, Switzerland) to ensure that the cornea is not damaged. If undamaged, the eye is further dissected from the head without damaging the eye or cornea. Care is taken to remove the eyeball from the orbit without cutting off the optical nerve too short. The enucleated eye is placed in a clamp (stainless steel clamp available from TNO, Zeist, the Netherlands) with the cornea positioned vertically and transferred to a chamber of the superfusion apparatus (TNO, Zeist). The clamp holding the eye is positioned in such a way that the entire cornea is supplied with isotonic saline from a bent stainless steel tube, at a rate of c. 0.10-0.15 ml/min (peristaltic pump, Desaga STA 131900, Heidelberg, Germany). The chambers of the superfusion apparatus and the saline are temperature-controlled at 32 +/- 1.5°C (water pump, Thermomix 1441, B.Braun Melsungen AG, Melsungen, Germany).

At least four eyes are selected, and, after being placed in the superfusion apparatus, are examined again with the slit-lamp microscope to ensure that they are not damaged. Corneal thickness is accurately measured at the corneal apex, using a Depth Measuring Device (Depth Measuring Attachment no. II for the Haag-Streit slit-lamp microscope) and is expressed in instrument units. Eyes with a corneal thickness deviating more than 10% from the mean value for the eyes, eyes that are unacceptably stained with fluorescein (score higher than 0.5, indicating the cornea to be permeable), or

eyes that show any other signs of damage, are rejected as test eyes and replaced.

After an equilibration period of 45-60 minutes, the corneal thickness of the eyes is measured again to determine the zero reference value for corneal swelling calculations. At time  $t = 0$ , i.e. immediately after the zero reference measurement, the test substance is applied to the eye. For this purpose, the clamp holding the eye is placed outside the chamber with the cornea facing upwards. Liquid materials are applied in amounts of 0.03 ml from a micropipette, in such a way that the entire surface of the cornea is bathed with the test substance. Solids, ground to a fine powder if necessary, are applied in an amount of 30 mg by powdering the entire surface of the cornea.

After an exposure period of 10 seconds, the corneal surface is rinsed thoroughly with 20 ml of isotonic saline at ambient temperature. The eye in the holder is then returned to its chamber. This procedure is repeated for each test eye. The test substance is tested on at least three eyes; one eye is treated in a similar way with isotonic saline only and serves as a control. The control eye and test eyes are examined at 30, 75, 120, 180 and 240 minutes after treatment, using the criteria and scoring system given in Annex 1. Fluorescein retention is only determined at 30 minutes after treatment. All examinations are carried out with the slit-lamp microscope and are noted on the scoring form given in Annex 2.

*N.B.. The dissection process can usually be mastered within a reasonable period, although some training will be required. The number of compounds that can be run on one day will depend on the number of chambers in the superfusion apparatus and on the number of eyes used to test each compound. The superfusion apparatus used at the TNO laboratory had eleven chambers and five eyes are used per compound, allowing two compounds to be run each day, with the eleventh eye serving as the control. Other laboratories use three test eyes per compound and thus can test three compounds per day. The number of tests can easily be increased if more chambers are available.*

*Annex 3 outlines the classification system used at TNO. A CEET Index was used to analyze data from the participating laboratories in the EEC/Colipa study. This was based on the addition of the maximum mean scores of corneal swelling, corneal opacity and fluorescein retention. The opacity and fluorescein scores were equally weighted in the index when compared to the maximum swelling % obtained. At TNO, the highest swelling observed is usually c. 60%, therefore the max. corneal opacity and fluorescein scores are multiplied by a factor of 20. This was used as the basis for the calculation of provisional CEET scores in the EEC/Colipa study. This way of scoring proved to be quite useful for statistical evaluation of the CEET results and for comparison with in vivo rabbit eye scores. However, it must be noted that the use of different sources for eyes and different thickness measurement devices may result in a variation in the obtained ranges of swelling. In such cases, a correction factor may need to be applied.*

## **ANNEX 1**

### **CRITERIA AND SCORING SYSTEM FOR CORNEAL EFFECTS**

The following criteria and scoring systems are applied for the assessment of possible effects:



**Corneal swelling**

Corneal swelling, expressed as a percentage, is calculated according to the following formula:

$$\frac{\text{corneal thickness at time } t - \text{corneal thickness at time } t = 0}{\text{corneal thickness at } t = 0} \times 100\%$$

The mean percentage of swelling for all test eyes is calculated for the observation time points of 30, 75, 120, 180 and 240 minutes.

**Corneal opacity**

Opacity degrees of density (the most dense area is used for scoring)

0 = no opacity

0.5 = very faint opacity

1 = scattered or diffuse areas, details of iris clearly visible

2 = easily discernible translucent area, details of iris slightly obscured

3 = severe corneal opacity, no specific details of iris visible, size of pupil barely discernible

4 = complete corneal opacity, iris invisible

The mean corneal opacity value for all test eyes is calculated for the observation time points of 30, 75, 120, 180 and 240 minutes.

**Fluorescein retention**

0 = no fluorescein retention

0.5 = very minor single cell staining

1 = single cell staining scattered throughout the treated area of the cornea

2 = focal or confluent dense single cell staining

3 = confluent large areas of the cornea retaining fluorescein

The mean fluorescein retention value for all test eyes is calculated for the observation time point of 30, minutes only. If desired, or in case of test substances that have adhered to the cornea, fluorescein retention can be determined at t = 240 min or whenever the test compound is removed.

*N.B.. In cases when all the test substance cannot be removed by the initial rinsing, further attempts to rinse it off are made at each observation time point.*

**Morphological effects**

These include "pitting" of corneal epithelial cells, "loosening" of epithelium, "roughening" of the corneal surface and "sticking" of the test substance to the cornea. These findings can vary in severity and they may occur simultaneously. The classification of these findings is subjective to the interpretation of the investigator.

**ANNEX 2****TNO NUTRITION - TOXICOLOGY AND NUTRITION INSTITUTE**

**ITV/IRR/006 F1**  
**TITLE: SCORING FORM CHICKEN ENUCLEATED EYE TEST (CEET)**

TEST COMPOUND: PROJECT NO.: DATE OF TESTING AND SIGNATURE:	LIQUID: <b>YES/NO</b> VISCOUS: <b>YES/NO</b> WARMED: <b>YES/NO</b> SOLID: <b>YES/NO</b> GROUND: <b>YES/NO</b> HYDROPHILIC/HYDROPHOBIC APPEARANCE:
---	--

EYE NO.	CORNEAL THICKNESS IN INSTRUMENT UNITS AT t =							CORNEAL OPACITY SCORES AT t =						OTHER EFFECTS	FLUORESCIN RETENTION	
	-45	0	30	75	120	180	240	0	30	75	120	180	240		0	30
actual time:->																
1																
sw%																
2																
sw%																
3																
sw%																
4																
sw%																
5																
sw%																
6																
sw%																
init. <sup>3</sup>																
mean <sup>1</sup>																
sem <sup>2</sup>																

CATEGORY :
CLASSIFICATION :

sw% = corneal swelling percentage; <sup>1</sup> = mean of the test eyes; <sup>2</sup> = standard error of the mean;

<sup>3</sup> = initials investigator; C = control eye (to be designated on the form)

REMARKS:

**ANNEX 3**

**TNO CLASSIFICATION SYSTEM APPLIED TO THE CHICKEN ENUCLEATED EYE TEST**

**1. SEVERITY OF EFFECTS**

On the basis of the severity of the observed findings for corneal swelling, corneal opacity and fluorescein retention, the effects are divided into four categories: I = none; II = slight; III = moderate; IV = severe.

Interpretation of corneal swelling, corneal opacity and fluorescein retention and classification into the four categories is done according to the following methodology:

**Corneal swelling (TNO classification)**

<i>mean corneal swelling %</i>	<i>category</i>
0 - 5	I
6 - 12	II
13 - 18 (>75 min. after treatment)	II
(<75 min. after treatment)	III
19 - 26	III
27 - 32 (>75 min. after treatment)	III
(<75 min. after treatment)	IV
32	IV

NOTE: This classification scheme is only applicable, if the range of swelling percentages obtained is approximately between 0% and 70%. Different slit lamp microscopes and depth measuring devices can give rise to a variation of the swelling range. Therefore, each laboratory must design a category system for corneal swelling using the principles described above, i.e. using the four categories: none, slight, moderate, severe.

**Corneal opacity**

---

<i>mean maximum opacity score</i>	<i>category</i>
<i>0.0 - 0.5</i>	<i>I</i>
<i>0.6 - 1.5</i>	<i>II</i>
<i>1.6 - 2.5</i>	<i>III</i>
<i>2.6 - 4.0</i>	<i>IV</i>

### **Fluorescein retention**

<i>mean fluorescein retention score at 30 min after treatment</i>	<i>category</i>
<i>0.0 - 0.5</i>	<i>I</i>
<i>0.6 - 1.5</i>	<i>II</i>
<i>1.6 - 2.5</i>	<i>III</i>
<i>2.6 - 4.0</i>	<i>IV</i>

## **2. ASSESSMENT OF THE *EX VIVO* EYE IRRITANCY CLASSIFICATION**

The *ex vivo* irritancy classification is assessed by reading the irritancy classification that corresponds to the combination of the category obtained for corneal swelling, corneal opacity and fluorescein retention, which are presented in the scheme below:

---

<i>Classification</i>	<i>Combination of the three categories</i>
<i>A. Not irritating</i>	3 x I 2 x I, 1 x II
<i>B. Slightly irritating</i>	3 x II 2 x II, 1 x I 2 x II, 1 x III 2 x I, 1 x IV <sup>1</sup> 1 x I, 1 x II, 1 x III <sup>1</sup>
<i>C. Moderately irritating</i>	3 x III 2 x III, 1 x II 2 x III, 1 x IV <sup>2</sup> 2 x III, 1 x I <sup>1</sup> 2 x II, 1 x IV <sup>1</sup> 1 x II, 1 x III, 1 x IV <sup>1</sup>
<i>D. Severely irritating</i>	3 x IV 2 x IV, 1 x III 2 x IV, 1 x II <sup>1</sup> 2 x IV, 1 x I <sup>1</sup> <b>immediate corneal opacity score 3</b> <b>corneal opacity score 4</b> <b>severe loosening of epithelium</b>

<sup>1</sup> Combinations of categories less likely to occur.

<sup>2</sup> Combination can be considered a borderline case between moderately and severely irritating.

Where considerable inter-eye variation is found, the compound should be retested.

### 3. EC-CLASSIFICATION OF EYE IRRITANTS AND EXTRAPOLATION FROM EX VIVO RESULTS TO EC-CLASSIFICATION

According to Directive 83/467/EEC, Part II (B) of Appendix 6, Dangerous Substances Directive, 5th Adaptation, the *in vivo* irritancy grades are divided into three classes, i.e. non-irritating (NI), irritating (R36) and severely irritating (R41). Extrapolation from the *ex vivo* irritancy grade to the EC-classification will be carried out using scientific judgement, redividing the original four categories into three. The combinations of the three categories that are allowed for each of the three classifications are mentioned in the scheme below.

<i>Classification</i>	<i>Combinations of the three categories</i>
<i>NI = not irritating (combination of A and B)</i>	3 x I 3 x II 2 x I, 1 x II 2 x II, 1 x I 1 x I, 1 x II, 1 x III <sup>1</sup>
<i>R36 = irritating (combination of B and C)</i>	3 x III 2 x II, 1 x III 2 x III, 1 x II 2 x III, 1 x IV 2 x I, 1 x IV <sup>1</sup> 2 x II, 1 x IV <sup>1</sup> 2 x III, 1 x I <sup>1</sup> 1 x II, 1 x III, 1 x IV <sup>1</sup>
<i>R41 = severely irritating</i>	3 x IV 2 x IV, 1 x III 2 x IV, 1 x II <sup>1</sup> 2 x IV, 1 x I <sup>1</sup> <b>immediate corneal opacity score 3</b> <b>corneal opacity score 4</b> <b>severe loosening of epithelium</b>

<sup>1</sup> Combinations of categories less likely to occur.

The combination of 3 x II can be considered as a borderline case between non-irritating and irritating.

The combination of 2 x III and 1 x IV can be considered as a borderline case between irritating and severely irritating.

**Table 1: An example of the use of the TNO classification system to predict irritancy** (data from Prinsen and Koëter, 1993)

<b>Test compound</b>	<b>Corneal swelling</b>	<b>Corneal opacity</b>	<b>Fluorescein retention</b>	<b>TNO classification</b>	<b>EC classification</b>
<i>Acetic acid</i>	<i>III</i>	<i>IV</i>	<i>IV</i>	<i>severe</i>	<i>R41</i>
<i>Brij 35</i>	<i>I</i>	<i>I</i>	<i>II</i>	<i>non</i>	<i>NI</i>
<i>Benzalkonium chloride</i>	<i>IV</i>	<i>IV</i>	<i>IV</i>	<i>severe</i>	<i>R41</i>
<i>Dimethyl sulphoxide</i>	<i>I</i>	<i>I</i>	<i>II</i>	<i>non</i>	<i>NI</i>
<i>Sodium fluorescein</i>	<i>I</i>	<i>I</i>	<i>I</i>	<i>non</i>	<i>NI</i>
<i>Glycerol</i>	<i>I</i>	<i>I</i>	<i>I</i>	<i>non</i>	<i>NI</i>
<i>Triacetin</i>	<i>I</i>	<i>I</i>	<i>I</i>	<i>non</i>	<i>NI</i>
<i>Mercury (II) chloride</i>	<i>IV</i>	<i>IV</i>	<i>III</i>	<i>severe</i>	<i>R41</i>
<i>Silver (I) nitrate</i>	<i>II</i>	<i>II</i>	<i>II</i>	<i>slight</i>	<i>NI</i>
<i>NaOH</i>	<i>IV</i>	<i>IV</i>	<i>IV</i>	<i>severe</i>	<i>R41</i>
<i>Toluene</i>	<i>I</i>	<i>II</i>	<i>II</i>	<i>slight</i>	<i>NI</i>
<i>Triethanolamine</i>	<i>I</i>	<i>II</i>	<i>II</i>	<i>slight</i>	<i>NI</i>
<i>n-Hexane</i>	<i>I</i>	<i>I</i>	<i>I</i>	<i>non</i>	<i>NI</i>
<i>Chloroform</i>	<i>III</i>	<i>II</i>	<i>III</i>	<i>moderate</i>	<i>R36</i>
<i>2-Methoxy ethanol</i>	<i>II</i>	<i>III</i>	<i>III</i>	<i>moderate</i>	<i>R36</i>
<i>1-Butanol</i>	<i>IV</i>	<i>III</i>	<i>IV</i>	<i>severe</i>	<i>R41</i>
<i>Acetaldehyde</i>	<i>III</i>	<i>II</i>	<i>III</i>	<i>moderate</i>	<i>R36</i>
<i>2-Butoxyethyl acetate</i>	<i>I</i>	<i>II</i>	<i>II</i>	<i>slight</i>	<i>NI</i>
<i>SDS</i>	<i>III</i>	<i>II</i>	<i>II</i>	<i>severe</i>	<i>R41</i>
<i>Dibutyltin dichloride</i>	<i>IV</i>	<i>III</i>	<i>IV</i>	<i>severe</i>	<i>R41</i>
<i>Tributyltin chloride</i>	<i>IV</i>	<i>III</i>	<i>IV</i>	<i>severe</i>	<i>R41</i>

N.B.. Silver (I) nitrate is a borderline case between NI and R36, 2-methoxy ethanol and acetaldehyde are borderline cases between R36 and R41, and SDS was upgraded from R36 to R41 because of an observed loosening of epithelium.

## References

Burton A.B.G. (1971)

A method for the objective assessment of eye irritation.  
**Food and Cosmetics Toxicol.** **10**: 209-217.

Burton A.B.G., York M., and Lawrence R.S. (1981)  
The *in vitro* assessment of severe irritants.  
**Food and Cosmetics Toxicol.** **19**: 471-480.

Commission of the European Communities (1991)  
Collaborative study on the evaluation of alternative methods to the eye irritation test.  
**EC Document XI/632/91, V/E/131/91.**

EEC standards (1983)  
EEC Directive 83/467/EEC  
**Official Journal of the European Communities, L 257, Volume 26.**

Methods for the determination of toxicity, B.5. Acute toxicity, eye irritation.  
**EEC Directive 84/449, Annex V** (September, 1984)

Jacobs G.A., and Martens M.A. (1990)  
Quantification of eye irritation based upon *in vitro* changes of corneal thickness.  
**ATLA 17**: 255-262.

Koëter H.B.W.M., and Prinsen M.K. (1985)  
Comparison of *in vivo* and *in vitro* eye irritancy test systems: A study with 34 substances.  
**Alternative Methods in Toxicology, Vol. 3**, Chapter A9  
Mary Ann Liebert Inc.; New York.

Mishima S. (1968)  
Corneal thickness.  
**Surv. Ophthalm.** **13**: 57-95.

Acute eye irritation/corrosion (1987)  
**OECD Guideline no. 405** (second updated version)  
Organization for Economic Co-operation and Development; Paris.

Price J.B., and Andrews I.J. (1985)  
The *in vitro* assessment of eye irritancy using isolated eyes.  
**Food and Chem. Toxicol.** **23**: 313-315.

Prinsen M.K., and Koëter H.B.W.M. (1990)  
EC-Validation study on alternatives to the Draize eye irritation test. Pilot interlaboratory comparison of the enucleated eye test.  
**TNO Report V89.464**, April 1990, Dept. Biol. Toxicol., TNO Toxicol. and Nutrition Institute, Zeist, The Netherlands.

Prinsen M.K., and Koëter H.B.W.M. (1992)  
Enucleated eye test with eyes of slaughterhouse animals as an alternative to the Draize eye irritation test with rabbits; a validation study with 21 reference compounds.  
**TNO Report V91.507**, February 1992, Dept. Biol. Toxicol., TNO Toxicol. and Nutrition Institute, Zeist, The Netherlands.



Prinsen M.K., and Koëter H.B.W.M. (1993)  
Justification of the enucleated eye test with eyes of slaughterhouse animals  
as an alternative to the Draize eye irritation test with rabbits.  
***Food and Chem. Toxicol.* 31: 69-76.**

*IP-80 copyright April, 1994*

***[This Page Intentionally Left Blank]***

## **Appendix A2**

### **Table of ICE Protocols**

***[This Page Intentionally Left Blank]***

<b>Test Method Component</b>	<b>Prinsen (2005)</b>	<b>Prinsen (2000)</b>	<b>Prinsen (1996)</b>	<b>Balls et al. (1995) (INVITTOX Protocol)</b>	<b>Prinsen and Koeter (1993)</b>
Time lapse from abattoir to test	≤ 2hr	≤ 2hr	≤ 2hr	≤ 2hr	≤ 2hr
Age of chicken	7 weeks	7 weeks	7 weeks	not specified	7 weeks
Weight of chicken	2.5-3.0 kg	2.5-3.0 kg	2.5-3.0 kg	not specified	2.5-3.0 kg
Number of eyes/ test material	3	3	5 or 3	at least 3	5
Corneal thickness deviation tolerance	>10% excluded	>10% excluded	>10% excluded	>10% excluded	>10% excluded
Length of equilibration period	45-60 min	45-60 min	45-60 min	45-60 min	45-60 min
Positive control	not included	not included	not included	not included	not included
Negative control	isotonic saline	isotonic saline	isotonic saline	isotonic saline	isotonic saline
Quantity applied	30 mL/30 mg	30 mL/30 mg	30 mL/30 mg	30 mL/30 mg	30 mL/30 mg
Exposure period	10 sec	10 sec	10 sec	10 sec	10 sec
Incubation temp	32±1.5°C	32±1.5°C	32±1.5°C	32±1.5°C	32±1.5°C
Perfusion rate	0.10-0.15 mL/min	0.10-0.15 mL/min	0.10-0.15 mL/min	0.10-0.15 mL/min	0.10-0.15 mL/min
Volume of rinse	20 mL saline	20 mL saline	20 mL saline	20 mL saline	20 mL saline
Slit lamp scope used	Haag-Streit scope	Haag-Streit scope	Haag-Streit scope	Haag-Streit scope	Haag-Streit scope
Evaluation times	0, 30, 75, 120, 180, 240 min PD	0, 30, 75, 120, 180, 240 min PD	0, 30, 75, 120, 180, 240 min PD	0, 30, 75, 120, 180, 240 min PD	0, 30, 75, 120, 180, 240 min PD

<b>Test Method Component</b>	<b>Prinsen (2005)</b>	<b>Prinsen (2000)</b>	<b>Prinsen (1996)</b>	<b>Balls et al. (1995) (INVITTOX Protocol)</b>	<b>Prinsen and Koeter (1993)</b>
Fluorescein observation time (2.0%)	30 min PD	30 min PD	30 min PD	30 min PD	30 min PD
Subjectivity of fluorescein evaluation	0-3 based on #cells retaining fluorescein	0-3 based on #cells retaining fluorescein	0-3 based on #cells retaining fluorescein	0-3 based on #cells retaining fluorescein	0-3 based on #cells retaining fluorescein
Subjectivity of corneal opacity	0-4 based on extent of opacification	0-4 based on extent of opacification	0-4 based on extent of opacification	0-4 based on extent of opacification	0-4 based on extent of opacification
Subjectivity of morphological findings	interpretation of investigator	interpretation of investigator	interpretation of investigator	interpretation of investigator	interpretation of investigator

<sup>1</sup>PD = Post dosing

## **Appendix B**

### **Chemical and Product Class Information for the Substances Tested in the ICE Test Method**

***[This Page Intentionally Left Blank]***



Substance	CASRN	Chemical Class	Product Class	Form Tested	Water Solubility <sub>1</sub>	Concentration Tested	Purity <sup>2</sup>
Acetaldehyde	75-07-0	Aldehyde	Manufacture of acetic acid, perfumes, and flavors; Narcotic	liquid	S	100%	99%
Acetic acid	64-19-7	Carboxylic acid	Reagent; Indicator	liquid	S	10%	99%
Acetone	67-64-1	Ketone	Solvent; Antiseptic; Chemical intermediate; Raw material	liquid	S	100%	99%
Ammonium nitrate	6484-52-2	Inorganic salt, Onium compound	Fertilizer; Chemical intermediate; Industrial explosive	solid	S	100%	>99.9%
L-Aspartic acid	70-47-3	Amino acid	Organic intermediate; Fungicides; Germicides	solid	S	100%	100%
Benzalkonium chloride (1%)	8001-54-5	Onium compound	Surfactant (cationic), Bactericide, Fungicide, Preservative	liquid	S	1, 5, 10 and 100%	98%
Brij 35	9002-92-0	Alcohol	Solvent; Excipient; Surfactant	n.p.	S	100%	n.p.
Butanol	71-36-3	Alcohol	Ingredient of spray paint; Nail polish	liquid	S	100%	99%
n-Butyl acetate	123-86-4	Ester	Solvent; Synthetic flavor ingredient	liquid	I *	100%	99%
2-Butoxyethyl acetate	112-07-2	Alcohol	Cleaner; Polish; Sealant	liquid	n.p.	100%	99%
Captan 90 concentrate	133-06-2	Imide, Organic sulfur compound	Pesticide	solid	S	100%	90%
4-Carboxybenzaldehyde	619-66-9	Carboxylic acid, Aldehyde	Manufacturing impurity (polyester); Developer intermediate	solid	I*	100%	95%
Cetylpyridinium bromide (0.1%)	140-72-7	Heterocyclic, Onium compound	Surfactant (cationic), Germicide, Laboratory reagent	liquid	Sf	0.1, 6 and 10%	98%
Chlorhexidine	55-56-1	Amine/Amidine	Disinfectant; Mouthwash; Anti-infective agent	solid	I*	100%	n.p.
Chloroform	67-66-3	Hydrocarbon (halogenated)	Solvent; Cleaner	liquid	I*	100%	99.8%
Cyclohexanol	108-93-0	Alcohol	Solvent; Chemical intermediate	liquid	S	100%	97%
Cyclohexylamino-functional PMS	—	Organosilicon compound	—	liquid	n.p.	—	n.p.

Substance	CASRN	Chemical Class	Product Class	Form Tested	Water Solubility <sup>1</sup>	Concentration Tested	Purity <sup>2</sup>
Decamethylcyclopentasiloxane	541-02-6	Organosilicon compound	Ingredient of hair conditioner; Diaper rash ointment; Car wax	liquid	n.p.	—	n.p.
Dibenzoyl-L-tartaric acid	2743-38-6	Carboxylic acid, Ester	Optical resolution agent	solid	I	100%	98%
Dibenzyl phosphate	1623-08-1	Ester, Organophosphorus compound	Not classified	solid	I*	100%	99%
Dibutyltin dichloride	683-18-1	Organometallic compound	Industrial chemical; Immunosuppressive agent	solid	S	100%	97%
2,6-Dichlorobenzoyl chloride	4659-45-4	Acyl halide	Anti-infective; Anti-fungal; Preservative	liquid	I*	100%	99%
2,2-Dimethylbutanoic acid	595-37-9	Carboxylic acid	Pharmaceutical metabolite	liquid	I	100%	96%
2,5-Dimethylhexanediol	110-03-2	Alcohol	Intermediate for pharmaceuticals; Pesticides; perfumes	solid	I	100%	99.5%
Dimethyl sulfoxide	67-68-5	Organic sulfur compound	Solvent; Cryoprotective agent	liquid	S	100%	99.9%
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent	liquid	S	100%	n.p.
Ethyl acetate	141-78-6	Ester	Solvent; Synthetic flavoring	liquid	S	100%	99%
2-Ethyl-1-hexanol	104-76-7	Alcohol	Solvent; Plasticizer	liquid	S	100%	99%
Ethyl-2-methylacetoacetate	609-14-3	Ketone, Ester	Not classified	liquid	S*	100%	97%
Ethyl trimethyl acetate	3938-95-2	Ester	Solvent	liquid	I*	100%	99%
Fomesafen	72128-02-0	Imide, Ether, Nitro compound	Pesticide	solid	S	100%	97.5%
Gammabutyrolactone	96-48-0	Heterocyclic, Lactone	Synthetic intermediate; Solvent	liquid	S	100%	>99%
Glycerol	56-81-5	Alcohol	Solvent; Plasticizer; Lubricant; Emollient; Drug vehicle	liquid	S	100%	>99%
n-Hexane	110-54-3	Hydrocarbon (acyclic)	Solvent; Adhesive; Gasoline additive	liquid	I	100%	99%
n-Hexanol	111-27-3	Alcohol	Solvent; Chemical intermediate; Synthetic flavor ingredient	liquid	I*	100%	98%
Imidazole	288-32-4	Heterocyclic	Anti-fungal; Enzyme inhibitor	solid	S	100%	99%

Substance	CASRN	Chemical Class	Product Class	Form Tested	Water Solubility <sub>1</sub>	Concentration Tested	Purity <sup>2</sup>
Isobutanol	78-83-1	Alcohol	Solvent; Chemical intermediate; Flavor ingredient	liquid	I*	100%	99.9%
Isopropanol	67-63-0	Alcohol	Solvent; Aerosol formulations (ingredient)	liquid	S	100%	99.9%
Maneb	12427-38-2	Amine/Amidine, Organic salt, Urea compound	Pesticide	solid	S	100%	90%
Mercury (II) chloride	7487-94-7	Inorganic chloride compound	Antiseptic; Disinfectant	solid	I	100%	99.5%
2-Methoxyethanol	109-86-4	Alcohol	Solvent	liquid	S	100%	99.9%
Methyl acetate	79-20-9	Ester	Solvent; Chemical intermediate; Synthetic flavor ingredient	liquid	S	100%	98%
Methyl cyanoacetate	105-34-0	Ester, Nitrile compound	Adhesive; Pharmaceutical intermediate	liquid	S*	100%	99%
Methyl ethyl ketone	78-93-3	Ketone	Solvent; Manufacture of lacquers, varnishes, cosmetics, pharmaceuticals	liquid	S	100%	99%
Methyl isobutyl ketone	108-10-1	Ketone	Solvent; Synthetic flavor; Drycleaning	liquid	I*	100%	98%
Methylcyclopentane	96-37-7	Hydrocarbon (cyclic)	Solvent	liquid	I*	100%	>99%
1-Naphthaleneacetic acid	86-87-3	Carboxylic acid, Polycyclic compound	Pesticide	solid	I*	100%	96%
1-Naphthaleneacetic acid, sodium salt	61-31-4	Carboxylic acid (salt), Polycyclic compound	Pesticide	solid	S*	100%	95%
n-Octanol	111-87-5	Alcohol	Solvent; Fragrance	liquid	I*	100%	>99%
Parafluoroaniline	371-40-4	Amine/Amidine	Intermediate for herbicides; Dyes	liquid	I	100%	99%
Polyethylene glycol 400	25322-68-3	Alcohol, Polyether	Surfactant (nonionic), Lubricant, Plasticizer, Solvent	liquid	S	100%	n.p.
Potassium cyanate	590-28-3	Inorganic salt	Herbicide; Pharmaceutical intermediate	solid	S	100%	97%
Promethazine HCl	58-33-3	Amine/Amidine, Heterocyclic, Organic sulfur compound	Antihistamine; Anti-nausea drug	solid	S*	100%	98%

Substance	CASRN	Chemical Class	Product Class	Form Tested	Water Solubility <sup>1</sup>	Concentration Tested	Purity <sup>2</sup>
Pyridine	110-86-1	Heterocyclic	Solvent; Intermediate for pharmaceuticals, dyes, pesticides	liquid	S	100%	>99.9%
Quinacrine	69-05-6	Amine/Amidine, Heterocyclic, Polycyclic compound	Anti-infective (anti-helmentic)	solid	S*	100%	n.p.
Silver (I) nitrate	7761-88-8	Inorganic silver/nitrogen compound	Anti-infective; Diagnostic agent	solid	S	3%	99%
Sodium dodecyl sulfate	151-21-3	Carboxylic acid (salt)	Surfactant (anionic), Detergent	solid	Sf	100%	70%
Sodium fluorescein	518-47-8	Polycyclic	Stain; Dye	liquid	S	20%	70.0%
Sodium hydroxide	1310-73-2	Alkali	Caustic agent	liquid	S	1%	n.p.
Sodium hydroxide	1310-73-2	Alkali	Caustic agent	liquid	S	1 and 10%	RG
Sodium lauryl sulfate	151-21-3	Carboxylic acid (salt)	Surfactant (anionic), Detergent	liquid	Sf	3 and 15%	98%
Sodium oxalate	62-76-0	Carboxylic acid (salt)	Textile finishing; Pyrotechnic, Industrial byproduct	solid	S	100%	>99%
Sodiumperborate, 4H <sub>2</sub> O	10486-00-7	Inorganic salt, Boron compound	Household cleaner; Detergent	solid	S	100%	98.6%
Tetraaminopyrimidine sulfate	5392-28-9	Amine/Amidine, Heterocyclic	Developer	solid	I*	100%	97%
TNO-01 (Formulation-1)	n.p.	Not classified	Not classified	liquid	n.p.	undiluted	n.p.
TNO-02 (Formulation-2)	n.p.	Not classified	Not classified	liquid	n.p.	undiluted	n.p.
TNO-03 (Pesticide-1)	n.p.	Not classified	Pesticide	liquid	n.p.	undiluted	n.p.
TNO-04 (Detergent-1 <sup>12</sup> )	n.p.	Not classified	Soaps; Surfactants	liquid	n.p.	undiluted	n.p.
TNO-05 (Silicone powder-1)	n.p.	Not classified	Not classified	solid	I	undiluted	n.p.
TNO-06 (Lubricant)	n.p.	Not classified	Not classified	gel	n.p.	undiluted	n.p.
TNO-07 (Ink-1)	n.p.	Not classified	Dyes	liquid	n.p.	undiluted	n.p.
TNO-08 (Ink-2)	n.p.	Not classified	Dyes	liquid	n.p.	undiluted	n.p.
TNO-09 (Paint)	n.p.	Not classified	Paint	liquid	n.p.	undiluted	n.p.
TNO-10 (Silicone powder-2)	n.p.	Not classified	Not classified	solid	I	undiluted	n.p.
TNO-11 (Sodium p-styrene sulfonate)	2695-37-6	Hydrocarbon; Acid	Industrial chemical	solid	n.p.	undiluted	n.p.
TNO-12 (Formulation-3)	n.p.	Not classified	Not classified	paste	n.p.	undiluted	n.p.
TNO-13 (Pesticide-2)	n.p.	Not classified	Pesticide	solid	n.p.	undiluted	n.p.
TNO-14 (Polydisaccharide)	n.p.	Carbohydrate	Not classified	liquid	n.p.	14.5%	n.p.
TNO-15 (Polydisaccharide)	n.p.	Carbohydrate	Not classified	liquid	n.p.	50%	n.p.
TNO-16 (Liquid nylon product)	n.p.	Not classified	Industrial formulation	liquid	n.p.	undiluted	n.p.
TNO-17 (Solvent-1)	n.p.	Not classified	Solvent	liquid	n.p.	undiluted	n.p.

Substance	CASRN	Chemical Class	Product Class	Form Tested	Water Solubility <sup>1</sup>	Concentration Tested	Purity <sup>2</sup>
TNO-18 (Solvent-2)	n.p.	Not classified	Solvent	liquid	n.p.	undiluted	n.p.
TNO-19 (Solvent-3)	n.p.	Not classified	Solvent	liquid	n.p.	undiluted	n.p.
TNO-20 (Solvent-4)	n.p.	Not classified	Solvent	liquid	n.p.	undiluted	n.p.
TNO-21 (Solvent-5)	n.p.	Not classified	Solvent	liquid	n.p.	undiluted	n.p.
TNO-22 (Solvent-6)	n.p.	Not classified	Solvent	liquid	n.p.	undiluted	n.p.
TNO-23 (Solvent-7)	n.p.	Not classified	Solvent	liquid	n.p.	undiluted	n.p.
TNO-24 (Solvent-8)	n.p.	Not classified	Solvent	liquid	n.p.	undiluted	n.p.
TNO-25 (Solvent-9)	n.p.	Not classified	Solvent	liquid	n.p.	undiluted	n.p.
TNO-26 (Ink-3)	n.p.	Not classified	Dyes	liquid	n.p.	undiluted	n.p.
TNO-27 (Thermal paper coating-1)	n.p.	Not classified	Industrial chemical	liquid	n.p.	undiluted	n.p.
TNO-28 (Toilet cleaner-1)	n.p.	Not classified	Household cleaner	liquid	n.p.	undiluted	n.p.
TNO-29 (Toilet cleaner-2)	n.p.	Not classified	Household cleaner	liquid	n.p.	undiluted	n.p.
TNO-30 (Pesticide-3)	n.p.	Not classified	Pesticide	solid	n.p.	undiluted	n.p.
TNO-31 (Sulfur)	7704-34-9	Inorganic chemical	Industrial chemical	solid	I	undiluted	n.p.
TNO-32 (Ink-4)	n.p.	Not classified	Dyes	liquid	n.p.	undiluted	n.p.
TNO-33 (Thermal paper coating-2)	n.p.	Not classified	Industrial chemical	liquid	n.p.	undiluted	n.p.
TNO-34 (Detergent-2)	n.p.	Not classified	Soaps; Surfactants	liquid	n.p.	undiluted	n.p.
TNO-35 (Propyl-lactate)	616-09-1	Acid	Food additive; Solvent	liquid	S	undiluted	n.p.
TNO-36 (Ethylhexyl lactate)	6283-86-9	Acid; Ester	Solvent; Wetting agent	liquid	n.p.	undiluted	n.p.
TNO-37 (Pesticide-4)	n.p.	Not classified	Pesticide	solid	n.p.	undiluted	n.p.
TNO-38 (Solvent-10)	n.p.	Not classified	Solvent	liquid	n.p.	undiluted	n.p.
TNO-39 (Detergent-3)	n.p.	Not classified	Soaps; Surfactants	liquid	n.p.	undiluted	n.p.
TNO-40 (Glycolbromoacetate form)	n.p.	Not classified	Not classified	liquid	n.p.	undiluted	n.p.
TNO-41 (Amidosulfonic acid)	5329-14-6	Acid	Herbicide; Flame retardant; Metal cleaning; Acid dye	solid	n.p.	100%	n.p.
TNO-42 (Glycolbromoacetate)	3785-34-0	Acetate	Not classified	liquid	n.p.	85%	n.p.
TNO-43 (Monobromoacetic acid)	79-08-3	Acid	Chlorination byproduct	solid	S	undiluted	n.p.
TNO-44 (Didecyldimethylammonium chloride [23% in propyl glycol])	7173-51-5	Not classified	Household cleaner (disinfectant)	liquid	n.p.	23%	n.p.
TNO-45 (Aqueous framing solution)	n.p.	Not classified	Not classified	liquid	n.p.	undiluted	n.p.
TNO-46 (Raw material powder)	n.p.	Not classified	Raw material	solid	n.p.	undiluted	n.p.
TNO-47 (Ferro powder)	n.p.	Not classified	Not classified	solid	n.p.	undiluted	n.p.
TNO-48 (Corrosion inhibitor liquid)	n.p.	Not classified	Not classified	liquid	n.p.	undiluted	n.p.
TNO-49 (Wood impregnator liquid)	n.p.	Not classified	Not classified	liquid	n.p.	undiluted	n.p.
TNO-50 (Sodium hypochlorite-containing formulation)	n.p.	Not classified	Disinfectant	n.p.	n.p.	undiluted	n.p.

Substance	CASRN	Chemical Class	Product Class	Form Tested	Water Solubility <sup>1</sup>	Concentration Tested	Purity <sup>2</sup>
TNO-51 (Disinfectant)	n.p.	Not classified	Disinfectant	n.p.	n.p.	undiluted	n.p.
TNO-52 (Pesticide liquid)	n.p.	Not classified	Pesticide	liquid	n.p.	undiluted	n.p.
TNO-53 (Ink formulation)	n.p.	Not classified	Dyes	liquid	n.p.	undiluted	n.p.
TNO-54 (Raw material powder)	n.p.	Not classified	Raw material	solid	n.p.	undiluted	n.p.
TNO-55 (Elastomer liquid)	n.p.	Not classified	Elastomer	liquid	n.p.	undiluted	n.p.
TNO-56 (Elastomer liquid)	n.p.	Not classified	Elastomer	liquid	n.p.	undiluted	n.p.
TNO-57 (Epoxy resin liquid)	n.p.	Not classified	Resin	liquid	n.p.	undiluted	n.p.
TNO-58 (Styrene resin powder)	n.p.	Not classified	Resin	solid	n.p.	undiluted	n.p.
TNO-59 (Ferro powder)	n.p.	Not classified	Not classified	solid	n.p.	undiluted	n.p.
TNO-60 (Fungicide paint)	n.p.	Not classified	Paint	liquid	n.p.	undiluted	n.p.
TNO-61 (Silver thiosulfate liquid)	n.p.	Not classified	Not classified	liquid	n.p.	undiluted	n.p.
TNO-62 (Lactate liquid)	n.p.	Not classified	Not classified	liquid	n.p.	undiluted	n.p.
TNO-63 (Copolymer powder)	n.p.	Not classified	Copolymer	solid	n.p.	undiluted	n.p.
TNO-64 (Fluoroallyl acrylate copolymer)	n.p.	Not classified	Copolymer	emulsion	n.p.	undiluted	n.p.
TNO-65 (Fluoroallyl acrylate copolymer)	n.p.	Not classified	Copolymer	emulsion	n.p.	undiluted	n.p.
TNO-66 (Raw material powder)	n.p.	Not classified	Raw material	solid	n.p.	undiluted	n.p.
TNO-67 (Ink formulation)	n.p.	Not classified	Dyes	liquid	n.p.	undiluted	n.p.
TNO-68 (Cleaning product)	n.p.	Not classified	Cleaner	liquid	n.p.	undiluted	n.p.
TNO-69 (Cleaning product)	n.p.	Not classified	Not classified	liquid	n.p.	2%	n.p.
TNO-70 (Fluoroallyl acrylate copolymer)	n.p.	Not classified	Copolymer	emulsion	n.p.	undiluted	n.p.
TNO-71 (Fluoroallyl acrylate copolymer)	n.p.	Not classified	Copolymer	emulsion	n.p.	undiluted	n.p.
TNO-72 (Fluoroallyl acrylate copolymer)	n.p.	Not classified	Copolymer	emulsion	n.p.	undiluted	n.p.
TNO-73 (Fluoroallyl acrylate copolymer)	n.p.	Not classified	Copolymer	emulsion	n.p.	undiluted	n.p.
TNO-74 (Raw material powder)	n.p.	Not classified	Raw material	solid	n.p.	undiluted	n.p.
TNO-75 (Fluoroallyl acrylate copolymer)	n.p.	Not classified	Copolymer	liquid	n.p.	undiluted	n.p.
TNO-76 (Ferro powder)	n.p.	Not classified	Not classified	solid	n.p.	undiluted	n.p.
TNO-77 (Raw material liquid)	n.p.	Not classified	Raw material	liquid	n.p.	undiluted	n.p.
TNO-78 (Raw material liquid)	n.p.	Not classified	Raw material	liquid	n.p.	undiluted	n.p.
TNO-79 (Silicon resin powder)	n.p.	Not classified	Silicone resin	solid	n.p.	undiluted	n.p.
TNO-80 (Raw material powder)	n.p.	Not classified	Raw material	solid	n.p.	undiluted	n.p.

Substance	CASRN	Chemical Class	Product Class	Form Tested	Water Solubility <sub>1</sub>	Concentration Tested	Purity <sup>2</sup>
TNO-81 (Surfactant liquid)	n.p.	Not classified	Soaps; Surfactants	liquid	n.p.	undiluted	n.p.
TNO-82 (Surfactant liquid)	n.p.	Not classified	Soaps; Surfactants	liquid	n.p.	undiluted	n.p.
TNO-83 (Surfactant liquid)	n.p.	Not classified	Soaps; Surfactants	liquid	n.p.	undiluted	n.p.
TNO-84 (Surfactant liquid)	n.p.	Not classified	Soaps; Surfactants	liquid	n.p.	undiluted	n.p.
TNO-85 (Surfactant liquid)	n.p.	Not classified	Soaps; Surfactants	liquid	n.p.	undiluted	n.p.
TNO-86 (Surfactant liquid)	n.p.	Not classified	Soaps; Surfactants	liquid	n.p.	undiluted	n.p.
TNO-87 (Enzyme liquid)	n.p.	Not classified	Enzyme solution	liquid	n.p.	undiluted	n.p.
TNO-88 (Miscellaneous liquid)	n.p.	Not classified	Not classified	liquid	n.p.	undiluted	n.p.
TNO-89 (Ferro powder)	n.p.	Not classified	Not classified	solid	n.p.	undiluted	n.p.
TNO-90 (Enzyme solution)	n.p.	Not classified	Enzyme solution	liquid	n.p.	undiluted	n.p.
TNO-91 (Enzyme solution)	n.p.	Not classified	Enzyme solution	liquid	n.p.	undiluted	n.p.
TNO-92 (Raw material powder)	n.p.	Not classified	Raw material	solid	n.p.	undiluted	n.p.
TNO-93 (Antifouling paint)	n.p.	Not classified	Paint	emulsion	n.p.	undiluted	n.p.
TNO-94 (Antifouling paint)	n.p.	Not classified	Paint	liquid	n.p.	undiluted	n.p.
Toluene	108-88-3	Hydrocarbon (cyclic)	Solvent; Gasoline additive; Manufacture of benzene derivatives, medicines, dyes, perfumes	liquid	I *	100%	99%
Triacetin	102-76-1	Lipid	Anti-fungal	liquid	I*	100%	99%
Tributyltin chloride	1461-22-9	Organometallic compound, Heavy metal	Pesticide; Preservative	liquid	n.p.	100%	96%
Trichloroacetic acid	76-03-9	Carboxylic acid	Caustic agent; Fixative; Herbicide	liquid	S	3 and 30%	RG
Triethanolamine	102-71-6	Amine/Amidine, Alcohol	Cleaner; Cosmetic ingredient; Intermediate for herbicides, waxes, cutting oils	liquid	S	100%	99.9%
Triton X-100	9002-93-1	Polyether	Surfactant (nonionic), Detergent, Emulsifier	liquid	Sf	5 and 10%	98%
Triton X-500	—	Polyether	Surfactant (nonionic), Detergent, Emulsifier	liquid	n.p.	5%	n.p.
Tween 20	9005-64-5	Ester, Polyether	Surfactant (nonionic), Detergent	liquid	Sf	100%	98%

<sup>1</sup>I=Insoluble, S=Soluble, Sf=Surfactant, \*=Solubility uncertain, n.p.=Not provided and not obtained

<sup>2</sup>n.p.=Not provided and not obtained, RG=Reagent grade



## **Appendix C**

### ***In Vitro* Data for Substances Tested in the ICE Assay**

<b>C1</b>	<b>ICE Data Sorted by Reference .....</b>	<b>C-3</b>
<b>C2</b>	<b>ICE Data Sorted by Substance Name .....</b>	<b>C-11</b>

***[This Page Intentionally Left Blank]***

## **Appendix C1**

### **ICE Data Sorted by Reference**

***[This Page Intentionally Left Blank]***

Substance/Product Name	CASRN	Form Tested	Water Solubility <sup>1</sup>	Concentration Tested	Purity	Source	Lab No.	Fluorescein Retention	Corneal Opacity	Corneal Swelling	In Vitro Classification (GHS)	Overall In Vitro Classification (GHS)	In Vitro Classification (EPA)	Overall In Vitro Classification (EPA)	In Vitro Classification (EU)	Overall In Vitro Classification (EU)	Reference
Acetone	67-64-1	liquid	S	undiluted	99%	Fisher	1	1.4	0.4	9.6	2B		III		NI		Balls et al. (1995)
Acetone	67-64-1	liquid	S	undiluted	99%	Fisher	2	1	1.7	49	2A	2A	II		R36	R36	Balls et al. (1995)
Acetone	67-64-1	liquid	S	undiluted	99%	Fisher	3	1.83	1.17	7.64	2B	2A	III		R36	R36	Balls et al. (1995)
Acetone	67-64-1	liquid	S	undiluted	99%	Fisher	4	3	1	13.8	2A	2A	II		R36	R36	Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	S	undiluted	>99.99%	Aldrich	1	1.2	0.9	6.7	2B		III		NI		Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	S	undiluted	>99.99%	Aldrich	2	2	1.3	42	2A	2B	II		R36	NI	Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	S	undiluted	>99.99%	Aldrich	3	1.33	1.5	12.33	2B		III		NI		Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	S	undiluted	>99.99%	Aldrich	4	2	0.5	6	2B		III		NI		Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	S	neat	100%	Degussa	1	1	0.7	3.2	2B		III		NI		Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	S	neat	100%	Degussa	2	2	2	56	2A	2A	II		R36	R36	Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	S	neat	100%	Degussa	3	1.83	1.67	14.67	2A		II		R36	R36	Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	S	neat	100%	Degussa	4	2	1	10	2B		III		R36	R36	Balls et al. (1995)
Benzalkonium chloride (1%)	8001-54-5	liquid	S	1%	98%	Sigma	1	1.8	0.6	18	2A/2B	2A	II/III		R36	R36	Balls et al. (1995)
Benzalkonium chloride (1%)	8001-54-5	liquid	S	1%	98%	Sigma	2	1.3	2.3	47	2A		II		R36	R36	Balls et al. (1995)
Benzalkonium chloride (1%)	8001-54-5	liquid	S	1%	98%	Sigma	3	2.67	1.5	12.66	2A		II		R36	R36	Balls et al. (1995)
Benzalkonium chloride (1%)	8001-54-5	liquid	S	1%	98%	Sigma	4	2	3	8.8	2A		II		R36	R36	Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	S	10%	98%	Sigma	1	3	3	37.7	1		I		R41	R41	Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	S	10%	98%	Sigma	2	3	2.3	95	1		I		R41	R41	Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	S	10%	98%	Sigma	3	3	2.33	40.72	1		I		R41	R41	Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	S	10%	98%	Sigma	4	3	2	41.1	1		I		R41	R41	Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	S	5%	98%	Sigma	1	3	2.6	36.3	1		I		R41	R41	Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	S	5%	98%	Sigma	2	1	2	42	2A		II		R36	R41	Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	S	5%	98%	Sigma	3	3	2	33.77	1		I		R41	R41	Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	S	5%	98%	Sigma	4	3	3	68.9	1		I		R41	R41	Balls et al. (1995)
n-Butyl acetate	123-86-4	liquid	I*	undiluted	99%	Fisher	1	1.8	1.8	13.9	2A		II		R36	R36	Balls et al. (1995)
n-Butyl acetate	123-86-4	liquid	I*	undiluted	99%	Fisher	2	0.5	2.7	42	1		I		R41	R36	Balls et al. (1995)
n-Butyl acetate	123-86-4	liquid	I*	undiluted	99%	Fisher	3	1	2	14.67	2A/2B	2A	II/III		R36	R36	Balls et al. (1995)
n-Butyl acetate	123-86-4	liquid	I*	undiluted	99%	Fisher	4	1	2	32.2	2A		II		R36	R36	Balls et al. (1995)
Gammabutyrolactone	96-48-0	liquid	S	undiluted	>99%	Aldrich	1	2.6	1.4	15.8	2A		II		R36	R36	Balls et al. (1995)
Gammabutyrolactone	96-48-0	liquid	S	undiluted	>99%	Aldrich	2	1.3	2	47	2A		II		R36	R36	Balls et al. (1995)
Gammabutyrolactone	96-48-0	liquid	S	undiluted	>99%	Aldrich	3	1.67	1.5	13.1	2A/2B		II/III		R36	R36	Balls et al. (1995)
Gammabutyrolactone	96-48-0	liquid	S	undiluted	>99%	Aldrich	4	1	2	13	2A/2B		II/III		R36	R36	Balls et al. (1995)
Captan 90 concentrate	133-06-2	solid	S	neat	90%	EPA	1	0	0.4	1.7	NI		IV		NI		Balls et al. (1995)
Captan 90 concentrate	133-06-2	solid	S	neat	90%	EPA	2	0.2	1	27	2B		III		NI/R36	NI	Balls et al. (1995)
Captan 90 concentrate	133-06-2	solid	S	neat	90%	EPA	3	0	1.33	19.17	2B		III		NI	NI	Balls et al. (1995)
Captan 90 concentrate	133-06-2	solid	S	neat	90%	EPA	4	1	1	20	2B		III		R36	R36	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	I*	neat	95%	Sigma	1	1	0.5	5.4	NI		IV		NI		Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	I*	neat	95%	Sigma	2	1.3	3	89	1		I		R41	NI	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	I*	neat	95%	Sigma	3	0.67	0.5	-1.4	NI		IV		NI	NI	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	I*	neat	95%	Sigma	4	2	1	12.7	2A/2B		II/III		R36	R36	Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	SF	0.1%	98%	Sigma	1	1	0	2.2	NI		IV		NI		Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	SF	0.1%	98%	Sigma	2	0.7	0	21	2B		III		NI	NI	Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	SF	0.1%	98%	Sigma	3	0.67	1	10.29	2B		III		NI	NI	Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	SF	0.1%	98%	Sigma	4	1	1	14.6	2B		III		NI/R36	NI	Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	liquid	SF	10%	98%	Sigma	1	2.6	1	25.8	2A		II		R36	R36	Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	liquid	SF	10%	98%	Sigma	2	1.7	2	41	2A		II		R36	R36	Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	liquid	SF	10%	98%	Sigma	3	2	1.67	27.2	2A		II		R36	R36	Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	liquid	SF	10%	98%	Sigma	4	3	3	17.8	1		I		R41	R36	Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	liquid	SF	6%	98%	Sigma	1	2	1.2	27.2	2A		II		R36	R36	Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	liquid	SF	6%	98%	Sigma	2	2	0.5	49	2A		II		R36	R36	Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	liquid	SF	6%	98%	Sigma	3	3	1.83	24.55	2A		II		R36	R36	Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	liquid	SF	6%	98%	Sigma	4	2.7	1.7	13.5	2A		II		R36	R36	Balls et al. (1995)
Chlorhexidine	55-56-1	solid	I*	neat	n.p.	Degussa	1	3	4	32	1		I		R41	R41	Balls et al. (1995)
Chlorhexidine	55-56-1	solid	I*	neat	n.p.	Degussa	2	3	4	150	1		I		R41	R41	Balls et al. (1995)
Chlorhexidine	55-56-1	solid	I*	neat	n.p.	Degussa	3	3	3	53.13	1		I		R41	R41	Balls et al. (1995)
Chlorhexidine	55-56-1	solid	I*	neat	n.p.	Degussa	4	3	4	-	1		I		R41	R41	Balls et al. (1995)
Cyclohexanol	108-93-0	liquid	S	undiluted	97%	Fisher	1	2.2	2.2	24.7	2A		II		R36	R36	Balls et al. (1995)
Cyclohexanol	108-93-0	liquid	S	undiluted	97%	Fisher	2	3	2	103	1		I		R41	R41	Balls et al. (1995)
Cyclohexanol	108-93-0	liquid	S	undiluted	97%	Fisher	3	3	2.5	35.74	1		I		R41	R41	Balls et al. (1995)
Cyclohexanol	108-93-0	liquid	S	undiluted	97%	Fisher	4	3	2.5	45.3	1		I		R41	R41	Balls et al. (1995)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	I	neat	98%	Aldrich	1	2.8	3	12.8	1		I		R41	R41	Balls et al. (1995)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	I	neat	98%	Aldrich	2	1	2.7	75	1		I		R41	R41	Balls et al. (1995)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	I	neat	98%	Aldrich	3	2	1.5	6.36	2B		III		R36	R41	Balls et al. (1995)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	I	neat	98%	Aldrich	4	1	2	6.7	2B		III		R36	R41	Balls et al. (1995)

Substance/Product Name	CASRN	Form Tested	Water Solubility <sup>1</sup>	Concentration Tested	Purity	Source	Lab No.	Fluorescein Retention	Corneal Opacity	Corneal Swelling	In Vitro Classification (GHS)	Overall In Vitro Classification (GHS)	In Vitro Classification (EPA)	Overall In Vitro Classification (EPA)	In Vitro Classification (EU)	Overall In Vitro Classification (EU)	Reference
Dibenzyl phosphate	1623-08-1	solid	I*	neat	99%	Aldrich	1	2.6	2	12.2	2A	2A/2B	II	II/III	R36	R36	Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	I*	neat	99%	Aldrich	2	1	0	22	2B		III		R36		Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	I*	neat	99%	Aldrich	3	2	1.5	17.07	2A/2B		II/III		R36		Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	I*	neat	99%	Aldrich	4	2	2	40.9	1		I		R36	Balls et al. (1995)	
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	I*	undiluted	99%	Aldrich	1	2.3	0.8	12.7	2A/2B	2A	II/III	II	R36	R36	Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	I*	undiluted	99%	Aldrich	2	2	1.3	26	2A		II		R36		Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	I*	undiluted	99%	Aldrich	3	1.83	1.67	17.15	2A		II		R36		Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	I*	undiluted	99%	Aldrich	4	1.8	0.8	16.8	2A/2B		II/III		R36	Balls et al. (1995)	
2,2-Dimethylbutanoic acid	595-37-9	liquid	I	undiluted	96%	Aldrich	1	3	2.4	43.8	1	1	I	I	R41	R41	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	I	undiluted	96%	Aldrich	2	3	2.7	74	1		I		R41		Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	I	undiluted	96%	Aldrich	3	3	2.5	35.9	1		I		R41		Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	I	undiluted	96%	Aldrich	4	3	3	62.7	1		I		R41	Balls et al. (1995)	
2,5-Dimethylhexanediol	110-03-2	solid	I	neat	99.5%	BASF	1	2	1	11.9	2B	2B	III	III	R36	R36	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	solid	I	neat	99.5%	BASF	2	3	3	64	1		I		R41		Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	solid	I	neat	99.5%	BASF	3	1.33	1.67	11.57	2B		III		R36		Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	solid	I	neat	99.5%	BASF	4	2	1	6.7	2B		III		R36	Balls et al. (1995)	
Ethanol	64-17-5	liquid	S	undiluted	n.p.	Local vendor	1	2.8	2.8	30.7	1	1	I	I	R41	R41	Balls et al. (1995)
Ethanol	64-17-5	liquid	S	undiluted	n.p.	Local vendor	2	2	3	74	1		I		R41		Balls et al. (1995)
Ethanol	64-17-5	liquid	S	undiluted	n.p.	Local vendor	3	2.5	2.33	35.88	2A		II		R36		Balls et al. (1995)
Ethanol	64-17-5	liquid	S	undiluted	n.p.	Local vendor	4	2	2.3	34.6	2A		II		R36	Balls et al. (1995)	
Ethyl acetate	141-78-6	liquid	S	undiluted	99%	Fisher	1	2	2	22	2A	2A	II	II	R36	R36	Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	S	undiluted	99%	Fisher	2	1.7	2.3	76	2A		II		R36		Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	S	undiluted	99%	Fisher	3	2	2	25.08	2A		II		R36		Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	S	undiluted	99%	Fisher	4	3	2	23	2A		II		R36	Balls et al. (1995)	
2-Ethyl-1-hexanol	104-76-7	liquid	S	undiluted	99%	Fisher	1	2	2.2	43	2A	2A	II	II	R36	R36	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	S	undiluted	99%	Fisher	2	1	2.3	62	2A		II		R36		Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	S	undiluted	99%	Fisher	3	3	1.5	13.31	2A		II		R36		Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	S	undiluted	99%	Fisher	4	1	2	52.4	2A		II		R36	Balls et al. (1995)	
Ethyl-2-methylacetoacetate	609-14-3	liquid	S*	undiluted	97%	Fluka	1	0.4	0.3	-2.8	NI	2B	IV	III	NI	NI	Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	S*	undiluted	97%	Fluka	2	1	0	7	2B		III		NI		Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	S*	undiluted	97%	Fluka	3	0.67	1	11.52	2B		III		NI		Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	S*	undiluted	97%	Fluka	4	1	0.5	4.5	NI		IV		NI	Balls et al. (1995)	
Ethyl trimethyl acetate	3938-95-2	liquid	I*	undiluted	99%	Aldrich	1	1.2	0.4	7.2	2B	2B	III	III	NI	NI	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	I*	undiluted	99%	Aldrich	2	2	2	31	2A		II		R36		Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	I*	undiluted	99%	Aldrich	3	0	0	1.44	NI		IV		NI		Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	I*	undiluted	99%	Aldrich	4	1	0.5	6.7	2B		III		NI	Balls et al. (1995)	
Fomesafen	72128-02-0	solid	S	neat	97.5%	EPA	1	0.9	1.2	5.3	2B	2B	III	III	NI	NI	Balls et al. (1995)
Fomesafen	72128-02-0	solid	S	neat	97.5%	EPA	2	0	0.2	11	NI		IV		NI		Balls et al. (1995)
Fomesafen	72128-02-0	solid	S	neat	97.5%	EPA	3	1	0.5	2.82	NI		IV		NI		Balls et al. (1995)
Fomesafen	72128-02-0	solid	S	neat	97.5%	EPA	4	1	1	4.3	2B		III		NI	Balls et al. (1995)	
Glycerol	56-81-5	liquid	S	undiluted	>99.5%	Mallinkrodt	1	1.2	1	5	2B	2B	III	III	NI	NI	Balls et al. (1995)
Glycerol	56-81-5	liquid	S	undiluted	>99.5%	Mallinkrodt	2	0	0	11	NI		IV		NI		Balls et al. (1995)
Glycerol	56-81-5	liquid	S	undiluted	>99.5%	Mallinkrodt	3	1.17	1	8.3	2B		III		NI		Balls et al. (1995)
Glycerol	56-81-5	liquid	S	undiluted	>99.5%	Mallinkrodt	4	2	0.5	29.4	2A		II		R36	Balls et al. (1995)	
n-Hexanol	111-27-3	liquid	I*	undiluted	98%	E-Kodak	1	2.8	1.6	17.4	2A	1	II	I	R36	R41	Balls et al. (1995)
n-Hexanol	111-27-3	liquid	I*	undiluted	98%	E-Kodak	2	0.2	1.7	82	2A		II		R36		Balls et al. (1995)
n-Hexanol	111-27-3	liquid	I*	undiluted	98%	E-Kodak	3	3	2.83	28.89	1		I		R41		Balls et al. (1995)
n-Hexanol	111-27-3	liquid	I*	undiluted	98%	E-Kodak	4	3	3	58.9	1		I		R41	Balls et al. (1995)	
Imidazole	288-32-4	solid	S	neat	99%	Aldrich	1	3	4	40.3	1	1	I	I	R41	R41	Balls et al. (1995)
Imidazole	288-32-4	solid	S	neat	99%	Aldrich	2	3	3	224	1		I		R41		Balls et al. (1995)
Imidazole	288-32-4	solid	S	neat	99%	Aldrich	3	3	2.5	36.96	1		I		R41		Balls et al. (1995)
Imidazole	288-32-4	solid	S	neat	99%	Aldrich	4	3	3	97.8	1		I		R41	Balls et al. (1995)	
Isobutanol	78-83-1	liquid	I*	undiluted	99.9%	Fisher	1	2.8	2.5	46.4	1	1	I	I	R41	R41	Balls et al. (1995)
Isobutanol	78-83-1	liquid	I*	undiluted	99.9%	Fisher	2	3	2.7	93	1		I		R41		Balls et al. (1995)
Isobutanol	78-83-1	liquid	I*	undiluted	99.9%	Fisher	3	3	2.5	37.06	1		I		R41		Balls et al. (1995)
Isobutanol	78-83-1	liquid	I*	undiluted	99.9%	Fisher	4	3	2	69.2	1		I		R41	Balls et al. (1995)	
Isopropanol	67-63-0	liquid	S	undiluted	99.9%	Fisher	1	2	1.6	23.3	2A	1	II	I	R36	R41	Balls et al. (1995)
Isopropanol	67-63-0	liquid	S	undiluted	99.9%	Fisher	2	0.7	2.7	72	1		I		R41		Balls et al. (1995)
Isopropanol	67-63-0	liquid	S	undiluted	99.9%	Fisher	3	3	2.5	37.84	1		I		R41		Balls et al. (1995)
Isopropanol	67-63-0	liquid	S	undiluted	99.9%	Fisher	4	2.3	0.5	8.9	2B		III		NI	Balls et al. (1995)	
Maneb	12427-38-2	solid	S	neat	90%	EPA	1	0	0.5	2.8	NI	NI	IV	IV	NI	NI	Balls et al. (1995)
Maneb	12427-38-2	solid	S	neat	90%	EPA	2	1	2	33	2A		II		R36		Balls et al. (1995)
Maneb	12427-38-2	solid	S	neat	90%	EPA	3	0	0.5	8.03	NI		IV		NI		Balls et al. (1995)
Maneb	12427-38-2	solid	S	neat	90%	EPA	4	1	1	6.7	2B		III		NI	Balls et al. (1995)	

Substance/Product Name	CASRN	Form Tested	Water Solubility <sup>1</sup>	Concentration Tested	Purity	Source	Lab No.	Fluorescein Retention	Corneal Opacity	Corneal Swelling	In Vitro Classification (GHS)	Overall In Vitro Classification (GHS)	In Vitro Classification (EPA)	Overall In Vitro Classification (EPA)	In Vitro Classification (EU)	Overall In Vitro Classification (EU)	Reference
Methyl acetate	79-20-9	liquid	S	undiluted	98%	Fisher	1	1.4	2.4	20.3	2A		II		R36		Balls et al. (1995)
Methyl acetate	79-20-9	liquid	S	undiluted	98%	Fisher	2	1	2.7	93	1	I	I	I	R41	R41	Balls et al. (1995)
Methyl acetate	79-20-9	liquid	S	undiluted	98%	Fisher	3	2	2	22.5	2A		II		R36		Balls et al. (1995)
Methyl acetate	79-20-9	liquid	S	undiluted	98%	Fisher	4	3	3	17.5	1		I		R41		Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	S*	undiluted	99%	Aldrich	1	0.4	0.3	4.5	NI		IV		NI		Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	S*	undiluted	99%	Aldrich	2	0.5	0.7	44	2A		II	IV	R36	NI	Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	S*	undiluted	99%	Aldrich	3	0.17	0.5	4.93	NI		IV		NI		Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	S*	undiluted	99%	Aldrich	4	1	1	10.7	2B		III		NI		Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	I*	undiluted	>99%	Fluka	1	0.4	0.5	2.3	NI		IV		NI		Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	I*	undiluted	>99%	Fluka	2	1	0	22	2B		III	IV	NI	NI	Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	I*	undiluted	>99%	Fluka	3	0	0.5	5.83	NI		IV		NI		Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	I*	undiluted	>99%	Fluka	4	1	0.5	0	NI		IV		NI		Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	S	undiluted	99%	Fisher	1	2	2.2	23.1	2A		II		R36		Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	S	undiluted	99%	Fisher	2	2.7	3	99	1		I	I	R41	R41	Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	S	undiluted	99%	Fisher	3	3	2.33	34.88	1		I		R41		Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	S	undiluted	99%	Fisher	4	3	2	12.6	2A		II		R36		Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	I*	undiluted	98%	Fisher	1	2.6	2	26.5	2A		II		R36		Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	I*	undiluted	98%	Fisher	2	3	3	64	1		I		R41		Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	I*	undiluted	98%	Fisher	3	2	2.17	21.69	2A	2A	II	II	R36	R36	Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	I*	undiluted	98%	Fisher	4	2	2	12.3	2A		II		R36		Balls et al. (1995)
1-Naphthaleneacetic acid	86-87-3	solid	I*	neat	96%	EPA	1	1	0.9	5.6	2B		III		NI		Balls et al. (1995)
1-Naphthaleneacetic acid	86-87-3	solid	I*	neat	96%	EPA	2	1	1	24	2B		III	III	R36	R36	Balls et al. (1995)
1-Naphthaleneacetic acid	86-87-3	solid	I*	neat	96%	EPA	3	2	1	8.86	2B		III		R36		Balls et al. (1995)
1-Naphthaleneacetic acid	86-87-3	solid	I*	neat	96%	EPA	4	1	1	46.7	2A		II		R36		Balls et al. (1995)
1-Naphthaleneacetic acid, sodium salt	61-31-4	solid	S*	neat	95%	EPA	1	3	3	46.6	1		I		R41		Balls et al. (1995)
1-Naphthaleneacetic acid, sodium salt	61-31-4	solid	S*	neat	95%	EPA	2	3	2.7	122	1		I	I	R41	R41	Balls et al. (1995)
1-Naphthaleneacetic acid, sodium salt	61-31-4	solid	S*	neat	95%	EPA	3	3	2.5	44.19	1		I		R41		Balls et al. (1995)
1-Naphthaleneacetic acid, sodium salt	61-31-4	solid	S*	neat	95%	EPA	4	3	3	64.1	1		I		R41		Balls et al. (1995)
n-Octanol	111-87-5	liquid	I*	undiluted	>99%	Aldrich	1	2	2.4	36.5	2A		II		R36		Balls et al. (1995)
n-Octanol	111-87-5	liquid	I*	undiluted	>99%	Aldrich	2	1.3	2	108	2A		II	II	R36	R36	Balls et al. (1995)
n-Octanol	111-87-5	liquid	I*	undiluted	>99%	Aldrich	3	1.17	1.5	10.18	2B		III		NI		Balls et al. (1995)
n-Octanol	111-87-5	liquid	I*	undiluted	>99%	Aldrich	4	2	1	25.7	2A		II		R36		Balls et al. (1995)
Paraffluoriline	371-40-4	liquid	I	undiluted	99%	Aldrich	1	3	2.2	35.3	1		I		R41		Balls et al. (1995)
Paraffluoriline	371-40-4	liquid	I	undiluted	99%	Aldrich	2	3	2	79	1		I	I	R41	R41	Balls et al. (1995)
Paraffluoriline	371-40-4	liquid	I	undiluted	99%	Aldrich	3	3	2	33.44	1		I		R41		Balls et al. (1995)
Paraffluoriline	371-40-4	liquid	I	undiluted	99%	Aldrich	4	3	2	38.5	1		I		R41		Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	SF	undiluted	n.p.	Aldrich	1	1.4	1	9.8	2B		III		NI		Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	SF	undiluted	n.p.	Aldrich	2	0.2	0	26	NI		IV		NI		Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	SF	undiluted	n.p.	Aldrich	3	2	1	5.88	2B		III	III	R36	R36	Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	SF	undiluted	n.p.	Aldrich	4	1	0.5	14.8	2B		III		R36		Balls et al. (1995)
Potassium cyanate	590-28-3	solid	S	neat	97%	Degussa	1	1	0.7	8	2B		III		NI		Balls et al. (1995)
Potassium cyanate	590-28-3	solid	S	neat	97%	Degussa	2	0.2	0	25	2B		III		NI		Balls et al. (1995)
Potassium cyanate	590-28-3	solid	S	neat	97%	Degussa	3	1.67	1	10.45	2B		III	III	R36	R36	Balls et al. (1995)
Potassium cyanate	590-28-3	solid	S	neat	97%	Degussa	4	1.3	1.7	25.3	2A		II		R36		Balls et al. (1995)
Promethazine HCl	58-33-3	solid	S*	neat	98%	Aldrich	1	2.6	1.6	33	1		I		R41		Balls et al. (1995)
Promethazine HCl	58-33-3	solid	S*	neat	98%	Aldrich	2	3	3	143	1		I		R41		Balls et al. (1995)
Promethazine HCl	58-33-3	solid	S*	neat	98%	Aldrich	3	3	2	23.02	2A		II	I	R36	R41	Balls et al. (1995)
Promethazine HCl	58-33-3	solid	S*	neat	98%	Aldrich	4	2	3	28.6	1/2A		I/II		R36/R41		Balls et al. (1995)
Pyridine	110-86-1	liquid	S	undiluted	>99.99%	Aldrich	1	3	2	32.7	1		I		R41		Balls et al. (1995)
Pyridine	110-86-1	liquid	S	undiluted	>99.99%	Aldrich	2	3	3	95	1		I		R41		Balls et al. (1995)
Pyridine	110-86-1	liquid	S	undiluted	>99.99%	Aldrich	3	3	2.5	37.47	1		I	I	R41	R41	Balls et al. (1995)
Pyridine	110-86-1	liquid	S	undiluted	>99.99%	Aldrich	4	3	3	78.6	1		I		R41		Balls et al. (1995)
Quinacrine	69-05-6	solid	S*	neat	n.p.	Sigma	1	1.2	0.6	4.1	2B		III		NI		Balls et al. (1995)
Quinacrine	69-05-6	solid	S*	neat	n.p.	Sigma	2	0.2	0.2	12	NI		IV	III	NI	NI	Balls et al. (1995)
Quinacrine	69-05-6	solid	S*	neat	n.p.	Sigma	3	2	2	11.49	2A		II		R36		Balls et al. (1995)
Quinacrine	69-05-6	solid	S*	neat	n.p.	Sigma	4	1	0.5	6.8	2B		III		NI		Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	liquid	S	1%	RG	Fisher	1	1	0.6	14.1	2B		III		NI/R36		Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	liquid	S	1%	RG	Fisher	2	0.7	2.3	55	2A		II	II	R36	R36	Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	liquid	S	1%	RG	Fisher	3	2.33	2.5	30.31	2A		II		R36		Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	liquid	S	1%	RG	Fisher	4	2	2	33.3	2A		II		R36		Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	S	10%	RG <sup>2</sup>	Fisher	1	3	4	32	1		I		R41		Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	S	10%	RG	Fisher	2	3	3.3	194	1		I		R41		Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	S	10%	RG	Fisher	3	3	3.17	68.86	1		I	I	R41	R41	Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	S	10%	RG	Fisher	4	3	4	151.7	1		I		R41		Balls et al. (1995)

Substance/Product Name	CASRN	Form Tested	Water Solubility <sup>1</sup>	Concentration Tested	Purity	Source	Lab No.	Fluorescein Retention	Corneal Opacity	Corneal Swelling	In Vitro Classification (GHS)	Overall In Vitro Classification (GHS)	In Vitro Classification (EPA)	Overall In Vitro Classification (EPA)	In Vitro Classification (EU)	Overall In Vitro Classification (EU)	Reference		
Sodium lauryl sulfate (15%)	151-21-3	liquid	SF	15%	98%	Sigma	1	0.6	0.4	7	2B	2B	III	III	NI	R36	Balls et al. (1995)		
Sodium lauryl sulfate (15%)	151-21-3	liquid	SF	15%	98%	Sigma	2	1	0.2	33	2A		II		R36		Balls et al. (1995)		
Sodium lauryl sulfate (15%)	151-21-3	liquid	SF	15%	98%	Sigma	3	1.67	1	9.56	2B		III		R36		Balls et al. (1995)		
Sodium lauryl sulfate (15%)	151-21-3	liquid	SF	15%	98%	Sigma	4	1	1	12.2	2B	2B	III	III	NI	NI	Balls et al. (1995)		
Sodium lauryl sulfate (3%)	151-21-3	liquid	SF	3%	98%	Sigma	1	1	0.2	3.9	NI		IV		NI		Balls et al. (1995)		
Sodium lauryl sulfate (3%)	151-21-3	liquid	SF	3%	98%	Sigma	2	0	0	39	2B		III		R36		NI	Balls et al. (1995)	
Sodium lauryl sulfate (3%)	151-21-3	liquid	SF	3%	98%	Sigma	3	1	0	2.75	NI	2B	IV	III	NI	NI	Balls et al. (1995)		
Sodium lauryl sulfate (3%)	151-21-3	liquid	SF	3%	98%	Sigma	4	1	1	15.9	2B		III		NI		Balls et al. (1995)		
Sodium oxalate	62-76-0	solid	S	neat	>99%	Aldrich	1	0.7	0.7	6.3	2B		III		NI		NI	Balls et al. (1995)	
Sodium oxalate	62-76-0	solid	S	neat	>99%	Aldrich	2	0.2	0	24	2B	2B	III	III	NI	NI	Balls et al. (1995)		
Sodium oxalate	62-76-0	solid	S	neat	>99%	Aldrich	3	0.5	0.5	2.62	NI		IV		NI		NI	Balls et al. (1995)	
Sodium oxalate	62-76-0	solid	S	neat	>99%	Aldrich	4	1	0	2.4	NI		IV		NI		NI	Balls et al. (1995)	
Sodium perborate, 4H <sub>2</sub> O	10486-00-7	solid	S	neat	98.6%	Dupont	1	0.6	0.5	3.1	NI	2B	IV	III	NI	NI	Balls et al. (1995)		
Sodium perborate, 4H <sub>2</sub> O	10486-00-7	solid	S	neat	98.6%	Dupont	2	0.2	0.7	23	2B		III		NI		NI	Balls et al. (1995)	
Sodium perborate, 4H <sub>2</sub> O	10486-00-7	solid	S	neat	98.6%	Dupont	3	1.33	1	7.54	2B		III		NI		NI	NI	Balls et al. (1995)
Sodium perborate, 4H <sub>2</sub> O	10486-00-7	solid	S	neat	98.6%	Dupont	4	1	0.5	14.6	2B	2B	III	III	NI	NI	Balls et al. (1995)		
Tetraaminopyrimidine sulfate	5392-28-9	solid	I*	neat	97%	Aldrich	1	1.3	1	7.5	2B		III		NI		NI	NI	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	I*	neat	97%	Aldrich	2	1	2	31	2A		II		R36		NI	Balls et al. (1995)	
Tetraaminopyrimidine sulfate	5392-28-9	solid	I*	neat	97%	Aldrich	3	1.5	1.5	7.3	2B	2B	III	III	NI	NI	Balls et al. (1995)		
Tetraaminopyrimidine sulfate	5392-28-9	solid	I*	neat	97%	Aldrich	4	1	1	8.9	2B		III		NI		NI	Balls et al. (1995)	
Toluene	108-88-3	liquid	I*	undiluted	99%	Fisher	2	1.4	1	5.2	2B		III		NI		NI	NI	Balls et al. (1995)
Toluene	108-88-3	liquid	I*	undiluted	99%	Fisher	3	2	1.3	29	2A	2A	II	II	R36	R36	Balls et al. (1995)		
Toluene	108-88-3	liquid	I*	undiluted	99%	Fisher	4	1.33	2	13.87	2A/2B		II/III		R36		NI	Balls et al. (1995)	
Toluene	108-88-3	liquid	I*	undiluted	99%	Fisher	1	1	2	58.2	2A		II		R36		NI	Balls et al. (1995)	
Trichloroacetic acid (3%)	76-03-9	liquid	S	3%	RG	Fisher	2	2.4	1.2	13.2	2A/2B	2A	II/III	II	R36	R36	Balls et al. (1995)		
Trichloroacetic acid (3%)	76-03-9	liquid	S	3%	RG	Fisher	3	2.3	2	38	2A		II		R36		NI	Balls et al. (1995)	
Trichloroacetic acid (3%)	76-03-9	liquid	S	3%	RG	Fisher	4	1.5	2.5	27.88	2A		II		R36		NI	Balls et al. (1995)	
Trichloroacetic acid (3%)	76-03-9	liquid	S	3%	RG	Fisher	1	1.7	2	26.4	2A	1	II	I	R36	R41	Balls et al. (1995)		
Trichloroacetic acid (30%)	76-03-9	liquid	S	30%	RG	Fisher	2	3	4	32	1		I		R41		NI	Balls et al. (1995)	
Trichloroacetic acid (30%)	76-03-9	liquid	S	30%	RG	Fisher	3	3	4	153	1		I		R41		NI	Balls et al. (1995)	
Trichloroacetic acid (30%)	76-03-9	liquid	S	30%	RG	Fisher	4	*	4	*	*	1	*	I	*	R41	Balls et al. (1995)		
Trichloroacetic acid (30%)	76-03-9	liquid	S	30%	RG	Fisher	1	3	4	*	1		I		R41		NI	Balls et al. (1995)	
Triton X-100 (10%)	9002-93-1	liquid	SF	10%	98%	Sigma	2	1.4	0.1	9.9	2B		III		NI		NI	NI	Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	SF	10%	98%	Sigma	3	1	0.8	29	2A/2B	2A/2B	II/III	II/III	R36	R36	Balls et al. (1995)		
Triton X-100 (10%)	9002-93-1	liquid	SF	10%	98%	Sigma	4	2.67	1.17	20.2	2A		II		R36		NI	Balls et al. (1995)	
Triton X-100 (10%)	9002-93-1	liquid	SF	10%	98%	Sigma	1	1.7	1	11.2	2B		III		R36		NI	Balls et al. (1995)	
Triton X-100 (5%)	9002-93-1	liquid	SF	5%	98%	Sigma	2	1	0.6	9.8	2B	2A	III	II	NI	R36	Balls et al. (1995)		
Triton X-100 (5%)	9002-93-1	liquid	SF	5%	98%	Sigma	3	1.3	0	38	2A		II		R36		NI	Balls et al. (1995)	
Triton X-100 (5%)	9002-93-1	liquid	SF	5%	98%	Sigma	4	2	0	3.97	2B		III		NI		NI	Balls et al. (1995)	
Triton X-100 (5%)	9002-93-1	liquid	SF	5%	98%	Sigma	1	1	2	39.6	2A	2B	II	III	R36	NI	Balls et al. (1995)		
Tween 20	9005-64-5	liquid	SF	undiluted	98%	Sigma	2	1	1	3.6	2B		III		NI		NI	NI	Balls et al. (1995)
Tween 20	9005-64-5	liquid	SF	undiluted	98%	Sigma	3	0.2	0	31	2B		III		NI		NI	NI	Balls et al. (1995)
Tween 20	9005-64-5	liquid	SF	undiluted	98%	Sigma	4	2.5	1	5.63	2B	2B	III	III	NI/R36	NI	Balls et al. (1995)		
Tween 20	9005-64-5	liquid	SF	undiluted	98%	Sigma	1	1	0.5	6.7	2B		III		R36		NI	Balls et al. (1995)	
TNO-01 (Formulation-1)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0	0	0	NI		NI		IV		IV	NI	NI
TNO-02 (Formulation-2)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	2.7	2	24	2A	2A	II	II	R36	R36	Prinsen (1996)		
TNO-03 (Pesticide-1)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.6	0.3	3	NI	NI	IV	IV	NI	NI	Prinsen (1996)		
TNO-04 (Detergent-1) <sup>10</sup>	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1.5	1.5	9	2B	2B	III	III	NI	NI	Prinsen (1996)		
TNO-05 (Silicone powder-1)	n.p.	solid	I	undiluted	n.p.	n.p.	-	0	0	0	NI	NI	IV	IV	NI	NI	Prinsen (1996)		
TNO-06 (Lubricant)	n.p.	gel	n.p.	undiluted	n.p.	n.p.	-	0	0	1	NI	NI	IV	IV	NI	NI	Prinsen (1996)		
TNO-07 (Ink-1)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.8	0	2	NI	NI	IV	IV	NI	NI	Prinsen (1996)		
TNO-08 (Ink-2)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.1	0	3	NI	NI	IV	IV	NI	NI	Prinsen (1996)		
TNO-09 (Paint)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1.3	0.5	5	NI	NI	IV	IV	NI	NI	Prinsen (1996)		
TNO-10 (Silicone powder-2)	n.p.	solid	I	undiluted	n.p.	n.p.	-	0	0	1	NI	NI	IV	IV	NI	NI	Prinsen (1996)		
TNO-11 (Sodium p-styrene sulfonate)	2695-37-6	solid	n.p.	undiluted	n.p.	n.p.	-	2	1.3	19	2A	2A	II	II	R36	R36	Prinsen (1996)		
TNO-12 (Formulation-3)	n.p.	paste	n.p.	undiluted	n.p.	n.p.	-	2.5	2	35	2A	2A	II	II	R36	R36	Prinsen (1996)		
TNO-13 (Pesticide-2)	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	0.7	0	1	NI	NI	IV	IV	NI	NI	Prinsen (1996)		
TNO-14 (Polysaccharide)	n.p.	liquid	n.p.	14.5%	n.p.	n.p.	-	0.3	0	2	NI	NI	IV	IV	NI	NI	Prinsen (1996)		
TNO-15 (Polysaccharide)	n.p.	liquid	n.p.	50%	n.p.	n.p.	-	0	0	2	NI	NI	IV	IV	NI	NI	Prinsen (1996)		
TNO-16 (Liquid nylon product)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0	0	1	NI	NI	IV	IV	NI	NI	Prinsen (1996)		
TNO-17 (Solvent-1)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.3	0	0	NI	NI	IV	IV	NI	NI	Prinsen (1996)		
TNO-18 (Solvent-2)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0	0	0	NI	NI	IV	IV	NI	NI	Prinsen (1996)		
TNO-19 (Solvent-3)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0	0	0	NI	NI	IV	IV	NI	NI	Prinsen (1996)		
TNO-20 (Solvent-4)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.5	0.3	3	NI	NI	IV	IV	NI	NI	Prinsen (1996)		
TNO-21 (Solvent-5)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.3	0.3	0	NI	NI	IV	IV	NI	NI	Prinsen (1996)		



Substance/Product Name	CASRN	Form Tested	Water Solubility <sup>1</sup>	Concentration Tested	Purity	Source	Lab No.	Fluorescein Retention	Corneal Opacity	Corneal Swelling	In Vitro Classification (GHS)	Overall In Vitro Classification (GHS)	In Vitro Classification (EPA)	Overall In Vitro Classification (EPA)	In Vitro Classification (EU)	Overall In Vitro Classification (EU)	Reference
TNO-22 (Solvent-6)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.2	0.3	0	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-23 (Solvent-7)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.2	0	2	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-24 (Solvent-8)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.2	0	3	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-25 (Solvent-9)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0	0	1	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-26 (Ink-3)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.1	0	0	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-27 (Thermal paper coating-1)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1	0.6	9	2B	2B	III	III	NI	NI	Prinsen (1996)
TNO-28 (Toilet cleaner-1)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1.4	0.8	12	2B	2B	III	III	NI	NI	Prinsen (1996)
TNO-29 (Toilet cleaner-2)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1.3	1	11	2B	2B	III	III	NI	NI	Prinsen (1996)
TNO-30 (Pesticide-3)	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	1.5	1	7	2B	2B	III	III	NI	NI	Prinsen (1996)
TNO-31 (Sulfur)	7704-34-9	solid	I	undiluted	n.p.	n.p.	-	0.2	0	1	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-32 (Ink-4)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1	0.5	7	2B	2B	III	III	NI	NI	Prinsen (1996)
TNO-33 (Thermal paper coating-2)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	2	0.5	5	2B	2B	III	III	NI	NI	Prinsen (1996)
TNO-34 (Detergent-2)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1	1	25	1	1	I	I	R41	R41	Prinsen (1996)
TNO-35 (Propyl-lactate)	616-09-1	liquid	S	undiluted	n.p.	n.p.	-	3	3	45	1	1	I	I	R41	R41	Prinsen (1996)
TNO-36 (Ethylhexyl lactate)	6283-86-9	liquid	n.p.	undiluted	n.p.	n.p.	-	2	2	18	2A	2A	II	II	R36	R36	Prinsen (1996)
TNO-37 (Pesticide-4)	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	1.5	1	15	2B	2B	III	III	NI	NI	Prinsen (1996)
TNO-38 (Solvent-10)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0	0	3	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-39 (Detergent-3)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.5	0.5	4	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-40 (Glycolbromoacetate form.)	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	2.6	1.9	41	1	I	I	I	R41	R41	Prinsen (1996)
TNO-41 (Amidosulfonic acid)	5329-14-6	solid	n.p.	undiluted	n.p.	n.p.	-	2.7	4	46	1	1	I	I	R41	R41	Prinsen (1996)
TNO-42 (Glycolbromoacetate)	3785-34-0	liquid	n.p.	85%	n.p.	n.p.	-	3	3	36	1	1	I	I	R41	R41	Prinsen (1996)
TNO-43 (Monobromoacetic acid)	79-08-3	solid	S	undiluted	n.p.	n.p.	-	3	4	80	1	1	I	I	R41	R41	Prinsen (1996)
TNO-44 (Didecyldimethylammoniumchloride (23% in propyl glycol))	7173-51-5	liquid	n.p.	23%	n.p.	n.p.	-	3	3.5	39	1	1	I	I	R41	R41	Prinsen (1996)
Cetylpyridinium bromide (6%)	—	liquid	Sf	undiluted	n.p.	n.p.	1	2.0	2.0	22	1	1	I	I	R41	R41	Prinsen (2000)
Cetylpyridinium bromide (6%)	—	liquid	Sf	undiluted	n.p.	n.p.	1	1.8	1.7	21	1	1	I	I	R41	R41	Prinsen (2000)
Cetylpyridinium bromide (6%)	—	liquid	Sf	undiluted	n.p.	n.p.	1	2.0	2.0	21	1	1	I	I	R41	R41	Prinsen (2000)
Cetylpyridinium bromide (6%)	—	liquid	Sf	undiluted	n.p.	n.p.	1	1.7	1.7	18	1	1	I	I	R41	R41	Prinsen (2000)
Cyclohexylamino-functional PMS	—	liquid	n.p.	undiluted	n.p.	n.p.	1	1.8	2.5	14	2A	2A	II	II	R36	R36	Prinsen (2000)
Cyclohexylamino-functional PMS	—	liquid	n.p.	undiluted	n.p.	n.p.	1	1.7	2.0	13	2A	2A	II	II	R36	R36	Prinsen (2000)
Cyclohexylamino-functional PMS	—	liquid	n.p.	undiluted	n.p.	n.p.	1	2.0	2.3	17	2A	2A	II	II	R36	R36	Prinsen (2000)
Cyclohexylamino-functional PMS	—	liquid	n.p.	undiluted	n.p.	n.p.	1	2.0	2.3	14	2A	2A	II	II	R36	R36	Prinsen (2000)
Cyclohexylamino-functional PMS	—	liquid	n.p.	undiluted	n.p.	n.p.	1	2.0	2.0	13	2A	2A	II	II	R36	R36	Prinsen (2000)
Decamethylcyclopentasiloxane	—	liquid	n.p.	undiluted	n.p.	n.p.	1	0.3	0.3	1	NI	NI	NI	NI	NI	NI	Prinsen (2000)
Decamethylcyclopentasiloxane	—	liquid	n.p.	undiluted	n.p.	n.p.	1	0.3	0.3	1	NI	NI	NI	NI	NI	NI	Prinsen (2000)
Decamethylcyclopentasiloxane	—	liquid	n.p.	undiluted	n.p.	n.p.	1	0.0	0.5	2	NI	NI	NI	NI	NI	NI	Prinsen (2000)
Decamethylcyclopentasiloxane	—	liquid	n.p.	undiluted	n.p.	n.p.	1	0.0	0.0	0	NI	NI	NI	NI	NI	NI	Prinsen (2000)
Decamethylcyclopentasiloxane	—	liquid	n.p.	undiluted	n.p.	n.p.	1	0.0	0.0	2	NI	NI	NI	NI	NI	NI	Prinsen (2000)
Triton X-500 (5%)	—	liquid	Sf	undiluted	n.p.	n.p.	1	1.0	0.7	14	2B	2B	III	III	NI	NI	Prinsen (2000)
Triton X-500 (5%)	—	liquid	Sf	undiluted	n.p.	n.p.	1	1.0	0.7	14	2B	2B	III	III	NI	NI	Prinsen (2000)
Triton X-500 (5%)	—	liquid	Sf	undiluted	n.p.	n.p.	1	1.0	0.7	13	2B	2B	III	III	NI	NI	Prinsen (2000)
Triton X-500 (5%)	—	liquid	Sf	undiluted	n.p.	n.p.	1	1.0	0.8	8	2B	2B	III	III	NI	NI	Prinsen (2000)
Triton X-500 (5%)	—	liquid	Sf	undiluted	n.p.	n.p.	1	1.0	0.7	11	2B	2B	III	III	NI	NI	Prinsen (2000)
TNO-45	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1	0.5	5	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-46	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	0	0	1	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-47	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	0	0	1	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-48	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	3	1	25	2A	2A	II	II	R36	R36	Prinsen (2005)
TNO-49	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	3	4	-	1	1	I	I	R41	R41	Prinsen (2005)
TNO-50	n.p.	n.p.	n.p.	undiluted	n.p.	n.p.	-	3	3	41.1	1	1	I	I	R41	R41	Prinsen (2005)
TNO-51	n.p.	n.p.	n.p.	undiluted	n.p.	n.p.	-	3	3	33.9	1	1	I	I	R41	R41	Prinsen (2005)
TNO-52	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1.7	1	5	2B	2B	III	III	NI	NI	Prinsen (2005)
TNO-53	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.5	0.2	3	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-54	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	1	1	9	2B	2B	III	III	NI	NI	Prinsen (2005)
TNO-55	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1.7	1.3	10	2B	2B	III	III	R36	R36	Prinsen (2005)
TNO-56	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	2	1.3	10	2B	2B	III	III	R36	R36	Prinsen (2005)
TNO-57	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1.5	1.3	12	2B	2B	III	III	NI	NI	Prinsen (2005)
TNO-58	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	0	0	-1	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-59	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	0.2	0	-2	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-60	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.2	0.5	1	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-61	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0	0	1	NI	NI	NI	NI	NI	NI	Prinsen (2005)

Substance/Product Name	CASRN	Form Tested	Water Solubility <sup>1</sup>	Concentration Tested	Purity	Source	Lab No.	Fluorescein Retention	Corneal Opacity	Corneal Swelling	In Vitro Classification (GHS)	Overall In Vitro Classification (GHS)	In Vitro Classification (EPA)	Overall In Vitro Classification (EPA)	In Vitro Classification (EU)	Overall In Vitro Classification (EU)	Reference
TNO-62	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	2	1	12	2B	2B	III	III	R36	R36	Prinsen (2005)
TNO-63	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	0.3	0.5	3	NI	NI	IV	IV	NI	NI	Prinsen (2005)
TNO-64	n.p.	emulsion	n.p.	undiluted	n.p.	n.p.	-	1	1	5	2B	2B	III	III	NI	NI	Prinsen (2005)
TNO-65	n.p.	emulsion	n.p.	undiluted	n.p.	n.p.	-	0.7	0.5	4	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-66	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	0	0	0	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-67	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1	1	6	2B	2B	III	III	NI	NI	Prinsen (2005)
TNO-68	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1/2	1	8	2A	2A	II	II	R36	R36	Prinsen (2005)
TNO-69	n.p.	liquid	n.p.	50%	n.p.	n.p.	-	1	0	0	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-70	n.p.	emulsion	n.p.	undiluted	n.p.	n.p.	-	2	1	20	2A	2A	II	II	R36	R36	Prinsen (2005)
TNO-71	n.p.	emulsion	n.p.	undiluted	n.p.	n.p.	-	1	0.5	13	2B	2B	III	III	NI	NI	Prinsen (2005)
TNO-72	n.p.	emulsion	n.p.	undiluted	n.p.	n.p.	-	1.5	0.5	5	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-73	n.p.	emulsion	n.p.	undiluted	n.p.	n.p.	-	2.7	2	18	1	1	1	1	R41	R41	Prinsen (2005)
TNO-74	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	0.5	0	0	NI	NI	IV	IV	NI	NI	Prinsen (2005)
TNO-75	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0	0	2	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-76	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	0	0	2	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-77	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1	0.5	7	2B	2B	III	III	NI	NI	Prinsen (2005)
TNO-78	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1.3	1	15	2B	2B	III	III	NI	NI	Prinsen (2005)
TNO-79	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	1	1	10	2B	2B	III	III	NI	NI	Prinsen (2005)
TNO-80	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	0.3	0	-1	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-81	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0	0	1	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-82	n.p.	n.p.	n.p.	undiluted	n.p.	n.p.	-	0	0	-2	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-83	n.p.	n.p.	n.p.	undiluted	n.p.	n.p.	-	0.8	0.7	10	2B	2B	III	III	NI	NI	Prinsen (2005)
TNO-84	n.p.	n.p.	n.p.	undiluted	n.p.	n.p.	-	0.7	0.7	2	2B	2B	III	III	NI	NI	Prinsen (2005)
TNO-85	n.p.	n.p.	n.p.	undiluted	n.p.	n.p.	-	2	1.3	14	2B	2B	III	III	R36	R36	Prinsen (2005)
TNO-86	n.p.	n.p.	n.p.	undiluted	n.p.	n.p.	-	1	1	7	2B	2B	III	III	NI	NI	Prinsen (2005)
TNO-87	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.7	1	1	2B	2B	III	III	NI	NI	Prinsen (2005)
TNO-88	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.3	0.7	3	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-89	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	0.2	0.7	1	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-90	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0	0	2	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-91	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0	0.2	1	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-92	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	0.8	1.7	16	2B	2B	III	III	R36	R36	Prinsen (2005)
TNO-93	n.p.	emulsion	n.p.	undiluted	n.p.	n.p.	-	3	2	17	2A	2A	II	II	R36	R36	Prinsen (2005)
TNO-94	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1	0.5	2	NI	NI	NI	NI	NI	NI	Prinsen (2005)
1-Butanol	71-36-3	liquid	S	undiluted	99%	Aldrich	-	2.9	2	54	1	1	1	1	R41	R41	Prinsen and Koeter (1993)
2-Butoxyethyl acetate	112-07-2	liquid	S	undiluted	99%	Aldrich	-	1	1	5	2B	2B	III	III	NI	NI	Prinsen and Koeter (1993)
2-Methoxyethanol	109-86-4	liquid	S	undiluted	99.9%	Aldrich	-	2	2	18	2A	2A	II	II	R36	R36	Prinsen and Koeter (1993)
Acetaldehyde	75-07-0	liquid	S	undiluted	99%	Aldrich	-	2	1.4	24	2A	2A	II	II	R36	R36	Prinsen and Koeter (1993)
Acetic acid	64-19-7	liquid	S	10%	99%	Aldrich	-	3	2.6	31	1	1	1	1	R41	R41	Prinsen and Koeter (1993)
Benzalkonium chloride (100%)	8001-54-5	liquid	S	undiluted	n.p.	Aldrich	-	3	3	40	1	1	1	1	R41	R41	Prinsen and Koeter (1993)
Brij 35	9002-92-0	liquid	S	undiluted	n.p.	Aldrich	-	0.9	0	5	NI	NI	IV	IV	NI	NI	Prinsen and Koeter (1993)
Chloroform	67-66-3	liquid	I*	undiluted	99.8%	Aldrich	-	2.5	1	21	2A	2A	II	II	R36	R36	Prinsen and Koeter (1993)
Dibutyltin dichloride	683-18-1	solid	S	undiluted	97%	Aldrich	-	3	2.5	34	1	1	1	1	R41	R41	Prinsen and Koeter (1993)
Dimethyl sulfoxide	67-68-5	liquid	S	undiluted	99.9%	Aldrich	-	1	0.5	4	NI	NI	IV	IV	NI	NI	Prinsen and Koeter (1993)
Glycerol	56-81-5	liquid	S	undiluted	99%	Aldrich	-	0.5	0.4	4	NI	NI	IV	IV	NI	NI	Prinsen and Koeter (1993)
Mercury (II) chloride	7487-94-7	solid	I	undiluted	99.5%	Aldrich	-	2	3.1	55	1	1	1	1	R41	R41	Prinsen and Koeter (1993)
n-Hexane	110-54-3	liquid	I	undiluted	99%	Aldrich	-	0.5	0	1	NI	NI	IV	IV	NI	NI	Prinsen and Koeter (1993)
Silver (I) nitrate	7761-88-8	solid	S	3%	99.5%	Aldrich	-	1	1	12	2B	2B	III	III	NI	NI	Prinsen and Koeter (1993)
Sodium dodecyl sulfate	151-21-3	solid	S	undiluted	70%	Aldrich	-	0.8	1	22	2B	2B	III	III	R41	R41	Prinsen and Koeter (1993)
Sodium fluorescein	518-47-8	liquid	S	20%	70% <sup>2</sup>	Aldrich	-	0.1	0	0	NI	NI	IV	IV	NI	NI	Prinsen and Koeter (1993)
Sodium hydroxide	1310-73-2	liquid	S	1%	97%	Aldrich	-	3	3	60	1	1	1	1	R41	R41	Prinsen and Koeter (1993)
Toluene	108-88-3	liquid	I*	undiluted	99.9%	Aldrich	-	1.1	1.4	4	2B	2B	III	III	NI	NI	Prinsen and Koeter (1993)
Triacetin	102-76-1	liquid	I*	undiluted	99%	Aldrich	-	0.5	0.4	4	NI	NI	IV	IV	NI	NI	Prinsen and Koeter (1993)
Tributyltin chloride	1461-22-9	liquid	n.p.	undiluted	96%	Aldrich	-	3	2.5	48	1	1	1	1	R41	R41	Prinsen and Koeter (1993)
Triethanolamine	102-71-6	liquid	S	undiluted	99%	Aldrich	-	0.9	0.7	4	2B	2B	III	III	NI	NI	Prinsen and Koeter (1993)

<sup>1</sup>S = Soluble: Sf = Surfactant: I = Insoluble: \*solubility uncertain

<sup>2</sup>RG = Reagent grade

<sup>3</sup>Numbering for substances from this reference assigned based on order of appearance in Table 3 of Prinsen (1996)

<sup>4</sup>Dve content

n.p. = Not provided and not obtained

## **Appendix C2**

### **ICE Data Sorted by Substance Name**

***[This Page Intentionally Left Blank]***





Substance/Product Name	CASRN	Form Tested	Water Solubility <sup>1</sup>	Concentration Tested	Purity	Source	Lab No.	Fluorescein Retention	Corneal Opacity	Corneal Swelling	In Vitro Classification (GHS)	Overall In Vitro Classification (GHS)	In Vitro Classification (EPA)	Overall In Vitro Classification (EPA)	In Vitro Classification (EU)	Overall In Vitro Classification (EU)	Reference
Glycerol	56-81-5	liquid	S	undiluted	>99.5%	Mallinkrodt	1	1.2	1	5	2B	2B	III	III	NI	NI	Balls et al. (1995)
Glycerol	56-81-5	liquid	S	undiluted	>99.5%	Mallinkrodt	2	0	0	11	NI	2B	IV	III	NI	NI	Balls et al. (1995)
Glycerol	56-81-5	liquid	S	undiluted	>99.5%	Mallinkrodt	3	1.17	1	8.3	2B	2B	III	III	NI	NI	Balls et al. (1995)
Glycerol	56-81-5	liquid	S	undiluted	>99.5%	Mallinkrodt	4	2	0.5	29.4	2A	2A	II	R36	NI	NI	Balls et al. (1995)
Glycerol	56-81-5	liquid	S	undiluted	99%	Aldrich	-	0.5	0.4	4	NI	NI	IV	IV	NI	NI	Prinsen and Koeter (1993)
n-Hexane	110-54-3	liquid	I	undiluted	99%	Aldrich	-	0.5	0	1	NI	NI	IV	IV	NI	NI	Prinsen and Koeter (1993)
n-Hexanol	111-27-3	liquid	I*	undiluted	98%	E-Kodak	1	2.8	1.6	17.4	2A	2A	II	R36	NI	NI	Balls et al. (1995)
n-Hexanol	111-27-3	liquid	I*	undiluted	98%	E-Kodak	2	0.2	1.7	82	2A	2A	II	R36	NI	NI	Balls et al. (1995)
n-Hexanol	111-27-3	liquid	I*	undiluted	98%	E-Kodak	3	3	2.83	28.89	1	1	I	R41	NI	NI	Balls et al. (1995)
n-Hexanol	111-27-3	liquid	I*	undiluted	98%	E-Kodak	4	3	3	58.9	1	1	I	R41	NI	NI	Balls et al. (1995)
Imidazole	288-32-4	solid	S	neat	99%	Aldrich	1	3	4	40.3	1	1	I	R41	NI	NI	Balls et al. (1995)
Imidazole	288-32-4	solid	S	neat	99%	Aldrich	2	3	3	224	1	1	I	R41	NI	NI	Balls et al. (1995)
Imidazole	288-32-4	solid	S	neat	99%	Aldrich	3	3	2.5	36.96	1	1	I	R41	NI	NI	Balls et al. (1995)
Imidazole	288-32-4	solid	S	neat	99%	Aldrich	4	3	3	97.8	1	1	I	R41	NI	NI	Balls et al. (1995)
Isobutanol	78-83-1	liquid	I*	undiluted	99.9%	Fisher	1	2.8	2.5	46.4	1	1	I	R41	NI	NI	Balls et al. (1995)
Isobutanol	78-83-1	liquid	I*	undiluted	99.9%	Fisher	2	3	2.7	93	1	1	I	R41	NI	NI	Balls et al. (1995)
Isobutanol	78-83-1	liquid	I*	undiluted	99.9%	Fisher	3	3	2.5	37.06	1	1	I	R41	NI	NI	Balls et al. (1995)
Isobutanol	78-83-1	liquid	I*	undiluted	99.9%	Fisher	4	3	2	69.2	1	1	I	R41	NI	NI	Balls et al. (1995)
Isopropanol	67-63-0	liquid	S	undiluted	99.9%	Fisher	1	2	1.6	23.3	2A	2A	II	R36	NI	NI	Balls et al. (1995)
Isopropanol	67-63-0	liquid	S	undiluted	99.9%	Fisher	2	0.7	2.7	72	1	1	I	R41	NI	NI	Balls et al. (1995)
Isopropanol	67-63-0	liquid	S	undiluted	99.9%	Fisher	3	3	2.5	37.84	1	1	I	R41	NI	NI	Balls et al. (1995)
Isopropanol	67-63-0	liquid	S	undiluted	99.9%	Fisher	4	2.3	0.5	8.9	2B	2B	III	NI	NI	Balls et al. (1995)	
Maneb	12427-38-2	solid	S	neat	90%	EPA	1	0	0.5	2.8	NI	NI	IV	IV	NI	NI	Balls et al. (1995)
Maneb	12427-38-2	solid	S	neat	90%	EPA	2	1	2	33	2A	2A	II	R36	NI	NI	Balls et al. (1995)
Maneb	12427-38-2	solid	S	neat	90%	EPA	3	0	0.5	8.03	NI	NI	IV	IV	NI	NI	Balls et al. (1995)
Maneb	12427-38-2	solid	S	neat	90%	EPA	4	1	1	6.7	2B	2B	III	NI	NI	NI	Balls et al. (1995)
Mercury (II) chloride	7487-94-7	solid	I	undiluted	99.5%	Aldrich	-	2	3.1	55	1	1	I	R41	NI	NI	Prinsen and Koeter (1993)
2-Methoxyethanol	109-86-4	liquid	S	undiluted	99.9%	Aldrich	-	2	2	18	2A	2A	II	R36	R36	R36	Prinsen and Koeter (1993)
Methyl acetate	79-20-9	liquid	S	undiluted	98%	Fisher	1	1.4	2.4	20.3	2A	2A	II	R36	NI	NI	Balls et al. (1995)
Methyl acetate	79-20-9	liquid	S	undiluted	98%	Fisher	2	1	2.7	93	1	1	I	R41	NI	NI	Balls et al. (1995)
Methyl acetate	79-20-9	liquid	S	undiluted	98%	Fisher	3	2	2	22.5	2A	2A	II	R36	NI	NI	Balls et al. (1995)
Methyl acetate	79-20-9	liquid	S	undiluted	98%	Fisher	4	3	3	17.5	1	1	I	R41	NI	NI	Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	S*	undiluted	99%	Aldrich	1	0.4	0.3	4.5	NI	NI	IV	IV	NI	NI	Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	S*	undiluted	99%	Aldrich	2	0.5	0.7	44	2A	2A	II	R36	NI	NI	Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	S*	undiluted	99%	Aldrich	3	0.17	0.5	4.93	NI	NI	IV	IV	NI	NI	Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	S*	undiluted	99%	Aldrich	4	1	1	10.7	2B	2B	III	NI	NI	NI	Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	I*	undiluted	>99%	Fluka	1	0.4	0.5	2.3	NI	NI	IV	IV	NI	NI	Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	I*	undiluted	>99%	Fluka	2	1	0	22	2B	2B	III	NI	NI	NI	Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	I*	undiluted	>99%	Fluka	3	0	0.5	5.83	NI	NI	IV	IV	NI	NI	Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	I*	undiluted	>99%	Fluka	4	1	0.5	0	NI	NI	IV	IV	NI	NI	Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	S	undiluted	99%	Fisher	1	2	2.2	23.1	2A	2A	II	R36	NI	NI	Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	S	undiluted	99%	Fisher	2	2.7	3	99	1	1	I	R41	NI	NI	Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	S	undiluted	99%	Fisher	3	3	2.33	34.88	1	1	I	R41	NI	NI	Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	S	undiluted	99%	Fisher	4	3	2	12.6	2A	2A	II	R36	NI	NI	Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	I*	undiluted	98%	Fisher	1	2.6	2	26.5	2A	2A	II	R36	NI	NI	Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	I*	undiluted	98%	Fisher	2	3	3	64	1	1	I	R41	NI	NI	Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	I*	undiluted	98%	Fisher	3	2	2.17	21.69	2A	2A	II	R36	NI	NI	Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	I*	undiluted	98%	Fisher	4	2	2	12.3	2A	2A	II	R36	NI	NI	Balls et al. (1995)
1-Naphthaleneacetic acid	86-87-3	solid	I*	neat	96%	EPA	1	1	0.9	5.6	2B	2B	III	NI	NI	NI	Balls et al. (1995)
1-Naphthaleneacetic acid	86-87-3	solid	I*	neat	96%	EPA	2	1	1	24	2B	2B	III	R36	NI	NI	Balls et al. (1995)
1-Naphthaleneacetic acid	86-87-3	solid	I*	neat	96%	EPA	3	2	1	8.86	2B	2B	III	R36	NI	NI	Balls et al. (1995)
1-Naphthaleneacetic acid	86-87-3	solid	I*	neat	96%	EPA	4	1	1	46.7	2A	2A	II	R36	NI	NI	Balls et al. (1995)
1-Naphthaleneacetic acid, sodium salt	61-31-4	solid	S*	neat	95%	EPA	1	3	3	46.6	1	1	I	R41	NI	NI	Balls et al. (1995)
1-Naphthaleneacetic acid, sodium salt	61-31-4	solid	S*	neat	95%	EPA	2	3	2.7	122	1	1	I	R41	NI	NI	Balls et al. (1995)
1-Naphthaleneacetic acid, sodium salt	61-31-4	solid	S*	neat	95%	EPA	3	3	2.5	44.19	1	1	I	R41	NI	NI	Balls et al. (1995)
1-Naphthaleneacetic acid, sodium salt	61-31-4	solid	S*	neat	95%	EPA	4	3	3	64.1	1	1	I	R41	NI	NI	Balls et al. (1995)
n-Octanol	111-87-5	liquid	I*	undiluted	>99%	Aldrich	1	2	2.4	36.5	2A	2A	II	R36	NI	NI	Balls et al. (1995)
n-Octanol	111-87-5	liquid	I*	undiluted	>99%	Aldrich	2	1.3	2	108	2A	2A	II	R36	NI	NI	Balls et al. (1995)
n-Octanol	111-87-5	liquid	I*	undiluted	>99%	Aldrich	3	1.17	1.5	10.18	2B	2B	III	NI	NI	NI	Balls et al. (1995)
n-Octanol	111-87-5	liquid	I*	undiluted	>99%	Aldrich	4	2	1	25.7	2A	2A	II	R36	NI	NI	Balls et al. (1995)
Paraffluoraniline	371-40-4	liquid	I	undiluted	99%	Aldrich	1	3	2.2	35.3	1	1	I	R41	NI	NI	Balls et al. (1995)
Paraffluoraniline	371-40-4	liquid	I	undiluted	99%	Aldrich	2	3	2	79	1	1	I	R41	NI	NI	Balls et al. (1995)
Paraffluoraniline	371-40-4	liquid	I	undiluted	99%	Aldrich	3	3	2	33.44	1	1	I	R41	NI	NI	Balls et al. (1995)
Paraffluoraniline	371-40-4	liquid	I	undiluted	99%	Aldrich	4	3	2	38.5	1	1	I	R41	NI	NI	Balls et al. (1995)







Substance/Product Name	CASRN	Form Tested	Water Solubility <sup>1</sup>	Concentration Tested	Purity	Source	Lab No.	Fluorescein Retention	Corneal Opacity	Corneal Swelling	In Vitro Classification (GHS)	Overall In Vitro Classification (GHS)	In Vitro Classification (EPA)	Overall In Vitro Classification (EPA)	In Vitro Classification (EU)	Overall In Vitro Classification (EU)	Reference
TNO-79	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	1	1	10	2B	2B	III	III	NI	NI	Prinsen (2005)
TNO-80	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	0.3	0	-1	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-81	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0	0	1	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-82	n.p.	n.p.	n.p.	undiluted	n.p.	n.p.	-	0	0	-2	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-83	n.p.	n.p.	n.p.	undiluted	n.p.	n.p.	-	0.8	0.7	10	2B	2B	III	III	NI	NI	Prinsen (2005)
TNO-84	n.p.	n.p.	n.p.	undiluted	n.p.	n.p.	-	0.7	0.7	2	2B	2B	III	III	NI	NI	Prinsen (2005)
TNO-85	n.p.	n.p.	n.p.	undiluted	n.p.	n.p.	-	2	1.3	14	2B	2B	III	III	R36	R36	Prinsen (2005)
TNO-86	n.p.	n.p.	n.p.	undiluted	n.p.	n.p.	-	1	1	7	2B	2B	III	III	NI	NI	Prinsen (2005)
TNO-87	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.7	1	1	2B	2B	III	III	NI	NI	Prinsen (2005)
TNO-88	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0.3	0.7	3	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-89	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	0.2	0.7	1	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-90	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0	0	2	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-91	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	0	0.2	1	NI	NI	NI	NI	NI	NI	Prinsen (2005)
TNO-92	n.p.	solid	n.p.	undiluted	n.p.	n.p.	-	0.8	1.7	16	2B	2B	III	III	R36	R36	Prinsen (2005)
TNO-93	n.p.	emulsion	n.p.	undiluted	n.p.	n.p.	-	3	2	17	2A	2A	II	II	R36	R36	Prinsen (2005)
TNO-94	n.p.	liquid	n.p.	undiluted	n.p.	n.p.	-	1	0.5	2	NI	NI	NI	NI	NI	NI	Prinsen (2005)
Toluene	108-88-3	liquid	I*	undiluted	99%	Fisher	2	1.4	1	5.2	2B						Balls et al. (1995)
Toluene	108-88-3	liquid	I*	undiluted	99%	Fisher	3	2	1.3	29	2A						Balls et al. (1995)
Toluene	108-88-3	liquid	I*	undiluted	99%	Fisher	4	1.33	2	13.87	2A/2B	2A	II				Balls et al. (1995)
Toluene	108-88-3	liquid	I*	undiluted	99%	Fisher	1	1	2	58.2	2A		II				Balls et al. (1995)
Toluene	108-88-3	liquid	I*	undiluted	99.9%	Aldrich	-	1.1	1.4	4	2B	2B	III	III	NI	NI	Prinsen and Koeter (1993)
Triacetin	102-76-1	liquid	I*	undiluted	99%	Aldrich	-	0.5	0.4	4	NI	NI	IV	IV	NI	NI	Prinsen and Koeter (1993)
Tributyltin chloride	1461-22-9	liquid	n.p.	undiluted	96%	Aldrich	-	3	2.5	48	1	1	I	I	R41	R41	Prinsen and Koeter (1993)
Trichloroacetic acid (3%)	76-03-9	liquid	S	3%	RG	Fisher	2	2.4	1.2	13.2	2A/2B		II/III				Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	S	3%	RG	Fisher	3	2.3	2	38	2A		II				Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	S	3%	RG	Fisher	4	1.5	2.5	27.88	2A	2A	II	II	R36	R36	Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	S	3%	RG	Fisher	1	1.7	2	26.4	2A		II				Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	S	30%	RG	Fisher	2	3	4	32	1		I				Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	S	30%	RG	Fisher	3	3	4	153	1		I				Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	S	30%	RG	Fisher	4	*	4	*	*		I	I	*	*	Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	S	30%	RG	Fisher	1	3	4	*	1		I				Balls et al. (1995)
Triethanolamine	102-71-6	liquid	S	undiluted	99%	Aldrich	-	0.9	0.7	4	2B	2B	III	III	NI	NI	Prinsen and Koeter (1993)
Triton X-500 (5%)	---	liquid	Sf	undiluted	n.p.	n.p.	1	1.0	0.7	14	2B		III				Prinsen (2000)
Triton X-500 (5%)	---	liquid	Sf	undiluted	n.p.	n.p.	1	1.0	0.7	14	2B		III				Prinsen (2000)
Triton X-500 (5%)	---	liquid	Sf	undiluted	n.p.	n.p.	1	1.0	0.7	13	2B		III	III	NI	NI	Prinsen (2000)
Triton X-500 (5%)	---	liquid	Sf	undiluted	n.p.	n.p.	1	1.0	0.8	8	2B		III				Prinsen (2000)
Triton X-500 (5%)	---	liquid	Sf	undiluted	n.p.	n.p.	1	1.0	0.7	11	2B		III				Prinsen (2000)
Triton X-100 (10%)	9002-93-1	liquid	Sf	10%	98%	Sigma	2	1.4	0.1	9.9	2B		III				Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	Sf	10%	98%	Sigma	3	1	0.8	29	2A/2B	2A/2B	II/III	II/III	R36	R36	Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	Sf	10%	98%	Sigma	4	2.67	1.17	20.2	2A		II				Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	Sf	10%	98%	Sigma	1	1.7	1	11.2	2B		III				Balls et al. (1995)
Triton X-100 (5%)	9002-93-1	liquid	Sf	5%	98%	Sigma	2	1	0.6	9.8	2B		III				Balls et al. (1995)
Triton X-100 (5%)	9002-93-1	liquid	Sf	5%	98%	Sigma	3	1.3	0	38	2A		II				Balls et al. (1995)
Triton X-100 (5%)	9002-93-1	liquid	Sf	5%	98%	Sigma	4	2	0	3.97	2B		III	II	NI	NI	Balls et al. (1995)
Triton X-100 (5%)	9002-93-1	liquid	Sf	5%	98%	Sigma	1	1	2	39.6	2A		II				Balls et al. (1995)
Tween 20	9005-64-5	liquid	Sf	undiluted	98%	Sigma	2	1	1	3.6	2B		III				Balls et al. (1995)
Tween 20	9005-64-5	liquid	Sf	undiluted	98%	Sigma	3	0.2	0	31	2B		III		NI/R36	NI	Balls et al. (1995)
Tween 20	9005-64-5	liquid	Sf	undiluted	98%	Sigma	4	2.5	1	5.63	2B		III	III	R36	R36	Balls et al. (1995)
Tween 20	9005-64-5	liquid	Sf	undiluted	98%	Sigma	1	1	0.5	6.7	2B		III		NI	NI	Balls et al. (1995)

<sup>1</sup>S = Soluble; Sf = Surfactant; I = Insoluble; \*solubility uncertain

<sup>2</sup>RG = Reagent grade

<sup>3</sup>Numbering for substances from this reference assigned based on order of appearance in Table 3 of Prinsen (1996)

<sup>4</sup>Dye content

n.p. = Not provided and not obtained

## **Appendix D**

### ***In Vivo and In Vitro* Comparison of Ocular Irritancy Classification**

**D-1 ICE Data Sorted by Reference ..... D-3**

**D-2 ICE Data Sorted by Substance Name ..... D-11**

***[This Page Intentionally Left Blank]***

## **Appendix D1**

### **ICE Data Sorted by Reference**

***[This Page Intentionally Left Blank]***

**In Vivo and In Vitro Comparison  
Sorted by Reference**

Substance/Product Name	CASRN	Concentration Tested	In Vitro Classification (GHS)	In Vivo Classification (GHS)	In Vitro Classification (EPA)	In Vivo Classification (EPA)	In Vitro Classification (EU)	In Vivo Classification (EU)	Reference
Acetone	67-64-1	undiluted	2A	2A	II	II	R36	R36	Balls et al. (1995)
Ammonium nitrate	6484-52-2	undiluted	2B	2B	III	III	NI	R36	Balls et al. (1995)
L-Aspartic acid	70-47-3	neat	2A	SCNM	II	SCNM	R36	SCNM	Balls et al. (1995)
Benzalkonium chloride (1%)	8001-54-5	1%	2A	I	II	I	R36	R41	Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	5%	I	I	I	I	R41	R41	Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	10%	I	I	I	I	R41	R41	Balls et al. (1995)
n-Butyl acetate	123-86-4	undiluted	2A	NI	II	III	R36	NI	Balls et al. (1995)
Gammabutyrolactone	96-48-0	undiluted	2A	2A	II	II	R36	R36	Balls et al. (1995)
Captan 90 concentrate	133-06-2	neat	2B	I	III	I	NI	R41	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	neat	NI	2A	IV	II	NI	R36	Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	0.1%	2B	NI	III	III	NI	NI	Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	6%	2A	I	II	SCNM	R36	R41	Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	10%	2A	I	II	I	R36	R41	Balls et al. (1995)
Chlorhexidine	55-56-1	neat	I	I	I	SCNM	R41	SCNM	Balls et al. (1995)
Cyclohexanol	108-93-0	undiluted	I	I	I	I	R41	R41	Balls et al. (1995)
Dibenzoyl-L-tartaric acid	2743-38-6	neat	I	I	I	SCNM	R41	R41	Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	neat	2A/2B	2A	II/III	II	R36	R36	Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	undiluted	2A	2A	II	II	R36	SCNM	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	undiluted	I	SCNM	I	I	R41	SCNM	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	neat	2B	I	III	I	R36	R41	Balls et al. (1995)
Ethanol	64-17-5	undiluted	I	2A	I	III	R41	NI	Balls et al. (1995)
Ethyl acetate	141-78-6	undiluted	2A	NI	II	III	R36	NI	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	undiluted	2A	2A	II	II	R36	R36	Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	undiluted	2B	2B	III	III	NI	NI	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	undiluted	2B	NI	III	III	NI	NI	Balls et al. (1995)
Fomesafen	72128-02-0	neat	2B	NI	III	III	NI	NI	Balls et al. (1995)
Glycerol	56-81-5	undiluted	2B	NI	III	IV	NI	NI	Balls et al. (1995)
n-Hexanol	111-27-3	undiluted	I	2A	I	II	R41	R36	Balls et al. (1995)
Imidazole	288-32-4	neat	I	I	I	I	R41	R41	Balls et al. (1995)
Isobutanol	78-83-1	undiluted	I	2A	I	II	R41	R36	Balls et al. (1995)
Isopropanol	67-63-0	undiluted	I	2A	I	III	R41	SCNM	Balls et al. (1995)
Maneb	12427-38-2	neat	NI	SCNM	IV	III	NI	SCNM	Balls et al. (1995)
Methyl acetate	79-20-9	undiluted	I	2A	I	II	R41	R36	Balls et al. (1995)
Methyl cyanoacetate	105-34-0	undiluted	NI	2A	IV	II	NI	R36	Balls et al. (1995)
Methylcyclopentane	96-37-7	undiluted	NI	NI	IV	III	NI	NI	Balls et al. (1995)
Methyl ethyl ketone	78-93-3	undiluted	I	2A	I	III	R41	R36	Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	undiluted	2A	NI	II	III	R36	NI	Balls et al. (1995)
1-Naphthaleneacetic acid	86-87-3	neat	2B	I	III	I	R36	SCNM	Balls et al. (1995)
1-Naphthaleneacetic acid, sodium salt	61-31-4	neat	I	I	I	I	R41	R41	Balls et al. (1995)
n-Octanol	111-87-5	undiluted	2A	2B	II	II	R36	R36	Balls et al. (1995)
Parafluoriline	371-40-4	undiluted	I	SCNM	I	SCNM	R41	SCNM	Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	undiluted	2B	NI	III	IV	R36	NI	Balls et al. (1995)
Potassium cyanate	590-28-3	neat	2B	SCNM	III	SCNM	R36	SCNM	Balls et al. (1995)
Promethazine HCl	58-33-3	neat	I	I	I	I	R41	R41	Balls et al. (1995)

**In Vivo and In Vitro Comparison**  
Sorted by Reference

Substance/Product Name	CASRN	Concentration Tested	In Vitro Classification (GHS)	In Vivo Classification (GHS)	In Vitro Classification (EPA)	In Vivo Classification (EPA)	In Vitro Classification (EU)	In Vivo Classification (EU)	Reference	
Pyridine	110-86-1	undiluted	1	1	I	I	R41	R41	Balls et al. (1995)	
Quinacrine	69-05-6	neat	2B	1	III	I	NI	R41	Balls et al. (1995)	
Sodium hydroxide (1%)	1310-73-2	1%	2A	2B	II	III	R36	R36	Balls et al. (1995)	
Sodium hydroxide (10%)	1310-73-2	10%	1	1	I	I	R41	R41	Balls et al. (1995)	
Sodium lauryl sulfate (3%)	151-21-3	3%	2B	NI	III	III	NI	NI	Balls et al. (1995)	
Sodium lauryl sulfate (15%)	151-21-3	15%	2B	1	III	I	R36	R36	Balls et al. (1995)	
Sodium oxalate	62-76-0	neat	2B	1	III	I	NI	R41	Balls et al. (1995)	
Sodium perborate, 4H <sub>2</sub> O	10486-00-7	neat	2B	1	III	I	NI	R41	Balls et al. (1995)	
Tetraaminopyrimidine sulfate	5392-28-9	neat	2B	NI	III	III	NI	NI	Balls et al. (1995)	
Toluene	108-88-3	undiluted	2A	NI	II	III	R36	NI	Balls et al. (1995)	
Trichloroacetic acid (3%)	76-03-9	3%	2A	NI	II	III	R36	NI	Balls et al. (1995)	
Trichloroacetic acid (30%)	76-03-9	30%	1	1	I	I	R41	R41	Balls et al. (1995)	
Triton X-100 (5%)	9002-93-1	5%	2A	2A	II	III	R36	NI	Balls et al. (1995)	
Triton X-100 (10%)	9002-93-1	10%	2A/2B	1	II/III	II	R36	R41	Balls et al. (1995)	
Tween 20	9005-64-5	undiluted	2B	NI	III	III	NI	NI	Balls et al. (1995)	
TNO-01 (Formulation-1)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)	
TNO-02 (Formulation-2)	n.p.	undiluted	2A	2A	II	II	R36	R36	Prinsen (1996)	
TNO-03 (Pesticide-1)	n.p.	undiluted	NI	NI	n.p.	IV	III	NI	NI	Prinsen (1996)
TNO-04 (Detergent-1)	n.p.	undiluted	2B	2A	III	III	NI	NI	Prinsen (1996)	
TNO-05 (Silicone powder-1)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)	
TNO-06 (Lubricant)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)	
TNO-07 (Ink-1)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)	
TNO-08 (Ink-2)	n.p.	undiluted	NI	NI	n.p.	IV	IV	NI	NI	Prinsen (1996)
TNO-09 (Paint)	n.p.	undiluted	NI	NI	IV	II	NI	NI	Prinsen (1996)	
TNO-10 (Silicone powder-2)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)	
TNO-11 (Sodium p-styrene sulfonate)	2695-37-6	undiluted	2A	SCNM	II	SCNM	R36	SCNM	Prinsen (1996)	
TNO-12 (Formulation-3)	n.p.	undiluted	2A	NI	II	SCNM	R36	R36	Prinsen (1996)	
TNO-13 (Pesticide-2)	n.p.	undiluted	NI	NI	n.p.	IV	IV	NI	NI	Prinsen (1996)
TNO-14 (Polydisaccharide)	n.p.	14.5%	NI	NI	IV	IV	NI	NI	Prinsen (1996)	
TNO-15 (Polydisaccharide)	n.p.	50%	NI	NI	IV	IV	NI	NI	Prinsen (1996)	
TNO-16 (Liquid nylon product)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)	
TNO-17 (Solvent-1)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)	
TNO-18 (Solvent-2)	n.p.	undiluted	NI	NI	n.p.	IV	IV	NI	NI	Prinsen (1996)
TNO-19 (Solvent-3)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)	
TNO-20 (Solvent-4)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)	
TNO-21 (Solvent-5)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)	
TNO-22 (Solvent-6)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)	
TNO-23 (Solvent-7)	n.p.	undiluted	NI	NI	n.p.	IV	IV	NI	NI	Prinsen (1996)
TNO-24 (Solvent-8)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)	
TNO-25 (Solvent-9)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)	
TNO-26 (Ink-3)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)	
TNO-27 (Thermal paper coating-1)	n.p.	undiluted	2B	2B	III	III	NI	NI	Prinsen (1996)	
TNO-28 (Toilet cleaner-1)	n.p.	undiluted	2B	1	III	I	NI	R41	Prinsen (1996)	
TNO-29 (Toilet cleaner-2)	n.p.	undiluted	2B	2A	III	III	NI	R36	Prinsen (1996)	



**In Vivo and In Vitro Comparison  
Sorted by Reference**

Substance/Product Name	CASRN	Concentration Tested	<i>In Vitro</i> Classification (GHS)	<i>In Vivo</i> Classification (GHS)	<i>In Vitro</i> Classification (EPA)	<i>In Vivo</i> Classification (EPA)	<i>In Vitro</i> Classification (EU)	<i>In Vivo</i> Classification (EU)	Reference
TNO-30 (Pesticide-3)	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (1996)
TNO-31 (Sulfur)	7704-34-9	undiluted	NI	NI	IV	III	NI	NI	Prinsen (1996)
TNO-32 (Ink-4)	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (1996)
TNO-33 (Thermal paper coating-2)	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (1996)
TNO-34 (Detergent-2)	n.p.	undiluted	1	SCNM	I	SCNM	R41	SCNM	Prinsen (1996)
TNO-35 (Propyl-lactate)	616-09-1	undiluted	1	1	I	I	R41	R41	Prinsen (1996)
TNO-36 (Ethylhexyl lactate)	6283-86-9	undiluted	2A	SCNM	II	II	R36	SCNM	Prinsen (1996)
TNO-37 (Pesticide-4)	n.p.	undiluted	2B	2B	III	III	NI	NI	Prinsen (1996)
TNO-38 (Solvent-10)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-39 (Detergent-3)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-40 (Glycolbromoacetate form.)	n.p.	undiluted	1	-	I	-	R41	R41 (SC)	Prinsen (1996)
TNO-41 (Amidosulfonic acid)	5329-14-6	undiluted	1	-	I	-	R41	R41 (SC)	Prinsen (1996)
TNO-42 (Glycolbromoacetate)	3785-34-0	85%	1	-	I	-	R41	R41 (SC)	Prinsen (1996)
TNO-43 (Monobromoacetic acid)	79-08-3	undiluted	1	-	I	-	R41	R41 (SC)	Prinsen (1996)
TNO-44 (Didecyldimethylammoniumchloride (23% in propyl glycol))	7173-51-5	23%	1	-	I	-	R41	R41 (SC)	Prinsen (1996)
Cetylpyridinium bromide (6%)	—	undiluted	1	1	I	SCNM	R41	R41	Prinsen (2000)
cyclohexylamino-functional PMS	—	undiluted	2A	-	II	-	R36	R36	Prinsen (2000)
decamethylcyclopentasiloxane	—	undiluted	NI	-	NI	-	NI	NI	Prinsen (2000)
Triton X-500 (5%)	—	undiluted	2B	-	III	-	NI	R36	Prinsen (2000)
TNO-45	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-46	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-47	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-48	n.p.	undiluted	2A	-	II	-	R36	R41 (SC)	Prinsen (2005)
TNO-49	n.p.	undiluted	1	-	I	-	R41	R41 (SC)	Prinsen (2005)
TNO-50	n.p.	undiluted	1	-	I	-	R41	R41 (SC)	Prinsen (2005)
TNO-51	n.p.	undiluted	1	-	I	-	R41	R41 (SC)	Prinsen (2005)
TNO-52	n.p.	undiluted	2B	2A	III	III	NI	R36	Prinsen (2005)
TNO-53	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-54	n.p.	undiluted	2B	2B	III	III	NI	NI	Prinsen (2005)
TNO-55	n.p.	undiluted	2B	2A	III	III	R36	R36	Prinsen (2005)
TNO-56	n.p.	undiluted	2B	2B	III	III	R36	NI	Prinsen (2005)
TNO-57	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (2005)
TNO-58	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-59	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-60	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-61	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-62	n.p.	undiluted	2B	NI	III	III	R36	NI	Prinsen (2005)
TNO-63	n.p.	undiluted	NI	NI	IV	III	NI	NI	Prinsen (2005)
TNO-64	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (2005)
TNO-65	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)

**In Vivo and In Vitro Comparison**  
Sorted by Reference

Substance/Product Name	CASRN	Concentration Tested	In Vitro Classification (GHS)	In Vivo Classification (GHS)	In Vitro Classification (EPA)	In Vivo Classification (EPA)	In Vitro Classification (EU)	In Vivo Classification (EU)	Reference
TNO-66	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-67	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (2005)
TNO-68	n.p.	undiluted	2A	2A	II	II	R36	R36	Prinsen (2005)
TNO-69	n.p.	50%	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-70	n.p.	undiluted	2A	2A	II	III	R36	R36	Prinsen (2005)
TNO-71	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (2005)
TNO-72	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-73	n.p.	undiluted	I	2A	I	II	R41	R36	Prinsen (2005)
TNO-74	n.p.	undiluted	NI	NI	IV	III	NI	NI	Prinsen (2005)
TNO-75	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-76	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-77	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (2005)
TNO-78	n.p.	undiluted	2B	2B	III	III	NI	NI	Prinsen (2005)
TNO-79	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (2005)
TNO-80	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-81	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-82	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-83	n.p.	undiluted	2B	2B	III	III	NI	R36	Prinsen (2005)
TNO-84	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (2005)
TNO-85	n.p.	undiluted	2B	I	III	I	R36	R41	Prinsen (2005)
TNO-86	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (2005)
TNO-87	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (2005)
TNO-88	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-89	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-90	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-91	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-92	n.p.	undiluted	2B	I	III	I	R36	R41	Prinsen (2005)
TNO-93	n.p.	undiluted	2A	I	II	I	R36	R41	Prinsen (2005)
TNO-94	n.p.	undiluted	NI	I	NI	I	NI	R41	Prinsen (2005)
1-Butanol	71-36-3	undiluted	I	2A	I	II	R41	R41	Prinsen and Koëter (1993)
2-Butoxyethyl acetate	112-07-2	undiluted	2B	-	III	-	NI	NI	Prinsen and Koëter (1993)
2-Methoxyethanol	109-86-4	undiluted	2A	-	II	-	R36	R36	Prinsen and Koëter (1993)
Acetaldehyde	75-07-0	undiluted	2A	-	II	-	R36	R36	Prinsen and Koëter (1993)
Acetic acid	64-19-7	10%	I	I	I	I	R41	R41	Prinsen and Koëter (1993)
Benzalkonium chloride (100%)	8001-54-5	undiluted	I	I	I	I	R41	R41	Prinsen and Koëter (1993)
Brij 35	9002-92-0	undiluted	NI	-	IV	-	NI	NI	Prinsen and Koëter (1993)
Chloroform	67-66-3	undiluted	2A	-	II	-	R36	R36	Prinsen and Koëter (1993)
Dibutyltin dichloride	683-18-1	undiluted	I	-	I	-	R41	R41	Prinsen and Koëter (1993)
Dimethyl sulfoxide	67-68-5	undiluted	NI	2B	IV	III	NI	NI	Prinsen and Koëter (1993)
Glycerol	56-81-5	undiluted	NI	NI	IV	IV	NI	NI	Prinsen and Koëter (1993)
Mercury (II) chloride	7487-94-7	undiluted	I	-	I	-	R41	R41	Prinsen and Koëter (1993)
n-Hexane	110-54-3	undiluted	NI	NI	IV	IV	NI	NI	Prinsen and Koëter (1993)
Silver (I) nitrate	7761-88-8	3%	2B	-	III	-	NI	NI	Prinsen and Koëter (1993)
Sodium dodecyl sulfate	151-21-3	undiluted	2B	-	III	-	R41	R41	Prinsen and Koëter (1993)

**In Vivo and In Vitro Comparison**  
Sorted by Reference

Substance/Product Name	CASRN	Concentration Tested	<i>In Vitro</i> Classification (GHS)	<i>In Vivo</i> Classification (GHS)	<i>In Vitro</i> Classification (EPA)	<i>In Vivo</i> Classification (EPA)	<i>In Vitro</i> Classification (EU)	<i>In Vivo</i> Classification (EU)	Reference
Sodium fluorescein	518-47-8	20%	NI	-	IV	-	NI	NI	Prinsen and Koëter (1993)
Sodium hydroxide	1310-73-2	1%	I	I	I	I	R41	R41	Prinsen and Koëter (1993)
Toluene	108-88-3	undiluted	2B	2B	III	III	NI	NI	Prinsen and Koëter (1993)
Triacetin	102-76-1	undiluted	NI	NI	IV	IV	NI	NI	Prinsen and Koëter (1993)
Tributyltin chloride	1461-22-9	undiluted	I	-	I	-	R41	R41	Prinsen and Koëter (1993)
Triethanolamine	102-71-6	undiluted	2B	NI	III	III	NI	NI	Prinsen and Koëter (1993)

SCNM - Study criteria not met

SC - Classification assigned on the basis of skin corrosion assay

***[This Page Intentionally Left Blank]***

## **Appendix D2**

### **ICE Data Sorted by Substance Name**

***[This Page Intentionally Left Blank]***

**In Vivo and In Vitro Data Comparison  
Sorted by Substance**

Substance/Product Name	CASRN	Concentration Tested	In Vitro Classification (GHS)	In Vivo Classification (GHS)	In Vitro Classification (EPA)	In Vivo Classification (EPA)	In Vitro Classification (EU)	In Vivo Classification (EU)	Reference
Acetaldehyde	75-07-0	undiluted	2A	-	II	-	R36	R36	Prinsen and Koeter (1993)
Acetic acid	64-19-7	10%	1	1	I	I	R41	R41	Prinsen and Koeter (1993)
Acetone	67-64-1	undiluted	2A	2A	II	II	R36	R36	Balls et al. (1995)
Ammonium nitrate	6484-52-2	undiluted	2B	2B	III	III	NI	R36	Balls et al. (1995)
L-Aspartic acid	70-47-3	neat	2A	SCNM	II	SCNM	R36	SCNM	Balls et al. (1995)
Benzalkonium chloride (1%)	8001-54-5	1%	2A	1	II	I	R36	R41	Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	5%	1	1	I	I	R41	R41	Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	10%	1	1	I	I	R41	R41	Balls et al. (1995)
Benzalkonium chloride (100%)	8001-54-5	undiluted	1	1	I	I	R41	R41	Prinsen and Koeter (1993)
Brij 35	9002-92-0	undiluted	NI	-	IV	-	NI	NI	Prinsen and Koeter (1993)
1-Butanol	71-36-3	undiluted	1	2A	I	II	R41	R41	Prinsen and Koeter (1993)
2-Butoxyethyl acetate	112-07-2	undiluted	2B	-	III	-	NI	NI	Prinsen and Koeter (1993)
n-Butyl acetate	123-86-4	undiluted	2A	NI	II	III	R36	NI	Balls et al. (1995)
gamma-Butyrolactone	96-48-0	undiluted	2A	2A	II	II	R36	R36	Balls et al. (1995)
Captan 90 concentrate	133-06-2	neat	2B	1	III	I	NI	R41	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	neat	NI	2A	IV	II	NI	R36	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	neat	NI	2A	IV	II	NI	R36	Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	0.1%	2B	NI	III	III	NI	NI	Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	6%	2A	1	II	SCNM	R36	R41	Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	undiluted	1	1	I	SCNM	R41	R41	Prinsen (2000)
Cetylpyridinium bromide (10%)	140-72-7	10%	2A	1	II	I	R36	R41	Balls et al. (1995)
Chlorhexidine	55-56-1	neat	1	1	I	SCNM	R41	SCNM	Balls et al. (1995)
Chloroform	67-66-3	undiluted	2A	-	II	-	R36	R36	Prinsen and Koeter (1993)
Cyclohexanol	108-93-0	undiluted	1	1	I	I	R41	R41	Balls et al. (1995)
Cyclohexylamino-functional PMS	—	undiluted	2A	-	II	-	R36	R36	Prinsen (2000)
Decamethylcyclopentasiloxane	—	undiluted	NI	-	NI	-	NI	NI	Prinsen (2000)
Dibenzoyl-L-tartaric acid	2743-38-6	neat	1	1	I	SCNM	R41	R41	Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	neat	2A/2B	2A	II/III	II	R36	R36	Balls et al. (1995)
Dibutyltin dichloride	683-18-1	undiluted	1	-	I	-	R41	R41	Prinsen and Koeter (1993)
2,6-Dichlorobenzoyl chloride	4659-45-4	undiluted	2A	2A	II	II	R36	SCNM	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	undiluted	1	SCNM	I	I	R41	SCNM	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	neat	2B	1	III	I	R36	R41	Balls et al. (1995)
Dimethyl sulfoxide	67-68-5	undiluted	NI	2B	IV	III	NI	NI	Prinsen and Koeter (1993)
Ethanol	64-17-5	undiluted	1	2A	I	III	R41	NI	Balls et al. (1995)
Ethyl acetate	141-78-6	undiluted	2A	NI	II	III	R36	NI	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	undiluted	2A	2A	II	II	R36	R36	Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	undiluted	2B	2B	III	III	NI	NI	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	undiluted	2B	NI	III	III	NI	NI	Balls et al. (1995)
Fomesafen	72128-02-0	neat	2B	NI	III	III	NI	NI	Balls et al. (1995)
Glycerol	56-81-5	undiluted	NI	NI	IV	IV	NI	NI	Prinsen and Koeter (1993)
n-Hexane	110-54-3	undiluted	NI	NI	IV	IV	NI	NI	Prinsen and Koeter (1993)
n-Hexanol	111-27-3	undiluted	1	2A	I	II	R41	R36	Balls et al. (1995)

**In Vivo and In Vitro Data Comparison  
Sorted by Substance**

Substance/Product Name	CASRN	Concentration Tested	In Vitro Classification (GHS)	In Vivo Classification (GHS)	In Vitro Classification (EPA)	In Vivo Classification (EPA)	In Vitro Classification (EU)	In Vivo Classification (EU)	Reference
Imidazole	288-32-4	neat	1	1	I	I	R41	R41	Balls et al. (1995)
Isobutanol	78-83-1	undiluted	1	2A	I	II	R41	R36	Balls et al. (1995)
Isopropanol	67-63-0	undiluted	1	2A	I	III	R41	SCNM	Balls et al. (1995)
Maneb	12427-38-2	neat	NI	SCNM	IV	III	NI	SCNM	Balls et al. (1995)
Mercury (II) chloride	7487-94-7	undiluted	1	-	I	-	R41	R41	Prinsen and Koëter (1993)
2-Methoxyethanol	109-86-4	undiluted	2A	-	II	-	R36	R36	Prinsen and Koëter (1993)
Methyl acetate	79-20-9	undiluted	1	2A	I	II	R41	R36	Balls et al. (1995)
Methyl cyanoacetate	105-34-0	undiluted	NI	2A	IV	II	NI	R36	Balls et al. (1995)
Methylcyclopentane	96-37-7	undiluted	NI	NI	IV	III	NI	NI	Balls et al. (1995)
Methyl ethyl ketone	78-93-3	undiluted	1	2A	I	III	R41	R36	Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	undiluted	2A	NI	II	III	R36	NI	Balls et al. (1995)
1-Naphthaleneacetic acid	86-87-3	neat	2B	1	III	I	R36	SCNM	Balls et al. (1995)
1-Naphthaleneacetic acid, sodium salt	61-31-4	neat	1	1	I	I	R41	R41	Balls et al. (1995)
n-Octanol	111-87-5	undiluted	2A	2B	II	II	R36	R36	Balls et al. (1995)
Parafluoranyliline	371-40-4	undiluted	1	SCNM	I	SCNM	R41	SCNM	Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	undiluted	2B	NI	III	IV	R36	NI	Balls et al. (1995)
Potassium cyanate	590-28-3	neat	2B	SCNM	III	SCNM	R36	SCNM	Balls et al. (1995)
Potassium cyanate	590-28-3	neat	2B	SCNM	III	SCNM	R36	SCNM	Balls et al. (1995)
Promethazine HCl	58-33-3	neat	1	1	I	I	R41	R41	Balls et al. (1995)
Pyridine	110-86-1	undiluted	1	1	I	I	R41	R41	Balls et al. (1995)
Quinacrine	69-05-6	neat	2B	1	III	I	NI	R41	Balls et al. (1995)
Silver (I) nitrate	7761-88-8	3%	2B	-	III	-	NI	NI	Prinsen and Koëter (1993)
Sodium dodecyl sulfate	151-21-3	undiluted	2B	-	III	-	R41	R41	Prinsen and Koëter (1993)
Sodium fluorescein	518-47-8	20%	NI	-	IV	-	NI	NI	Prinsen and Koëter (1993)
Sodium hydroxide	1310-73-2	1%	1	1	I	I	R41	R41	Prinsen and Koëter (1993)
Sodium hydroxide (1%)	1310-73-2	1%	2A	2B	II	III	R36	R36	Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	10%	1	1	I	I	R41	R41	Balls et al. (1995)
Sodium lauryl sulfate (3%)	151-21-3	3%	2B	NI	III	III	NI	NI	Balls et al. (1995)
Sodium lauryl sulfate (15%)	151-21-3	15%	2B	1	III	I	R36	R36	Balls et al. (1995)
Sodium oxalate	62-76-0	neat	2B	1	III	I	NI	R41	Balls et al. (1995)
Sodium perborate, 4H <sub>2</sub> O	10486-00-7	neat	2B	1	III	I	NI	R41	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	neat	2B	NI	III	III	NI	NI	Balls et al. (1995)
TNO-01 (Formulation-1)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-02 (Formulation-2)	n.p.	undiluted	2A	2A	II	II	R36	R36	Prinsen (1996)
TNO-03 (Pesticide-1)	n.p.	undiluted	NI	NI	IV	III	NI	NI	Prinsen (1996)
TNO-04 (Detergent-1 <sup>3</sup> )	n.p.	undiluted	2B	2A	III	III	NI	NI	Prinsen (1996)
TNO-05 (Silicone powder-1)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-06 (Lubricant)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-07 (Ink-1)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-08 (Ink-2)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-09 (Paint)	n.p.	undiluted	NI	NI	IV	II	NI	NI	Prinsen (1996)
TNO-10 (Silicone powder-2)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)



**In Vivo and In Vitro Data Comparison  
Sorted by Substance**

Substance/Product Name	CASRN	Concentration Tested	In Vitro Classification (GHS)	In Vivo Classification (GHS)	In Vitro Classification (EPA)	In Vivo Classification (EPA)	In Vitro Classification (EU)	In Vivo Classification (EU)	Reference
TNO-11 (Sodium p-styrene sulfonate)	2695-37-6	undiluted	2A	SCNM	II	SCNM	R36	SCNM	Prinsen (1996)
TNO-12 (Formulation-3)	n.p.	undiluted	2A	NI	II	SCNM	R36	R36	Prinsen (1996)
TNO-13 (Pesticide-2)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-14 (Polydisaccharide)	n.p.	14.5%	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-15 (Polydisaccharide)	n.p.	50%	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-16 (Liquid nylon product)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-17 (Solvent-1)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-18 (Solvent-2)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-19 (Solvent-3)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-20 (Solvent-4)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-21 (Solvent-5)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-22 (Solvent-6)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-23 (Solvent-7)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-24 (Solvent-8)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-25 (Solvent-9)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-26 (Ink-3)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-27 (Thermal paper coating-1)	n.p.	undiluted	2B	2B	III	III	NI	NI	Prinsen (1996)
TNO-28 (Toilet cleaner-1)	n.p.	undiluted	2B	I	III	I	NI	R41	Prinsen (1996)
TNO-29 (Toilet cleaner-2)	n.p.	undiluted	2B	2A	III	III	NI	R36	Prinsen (1996)
TNO-30 (Pesticide-3)	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (1996)
TNO-31 (Sulfur)	7704-34-9	undiluted	NI	NI	IV	III	NI	NI	Prinsen (1996)
TNO-32 (Ink-4)	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (1996)
TNO-33 (Thermal paper coating-2)	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (1996)
TNO-34 (Detergent-2)	n.p.	undiluted	I	SCNM	I	SCNM	R41	SCNM	Prinsen (1996)
TNO-35 (Propyl-lactate)	616-09-1	undiluted	I	I	I	I	R41	R41	Prinsen (1996)
TNO-36 (Ethylhexyl lactate)	6283-86-9	undiluted	2A	SCNM	II	II	R36	SCNM	Prinsen (1996)
TNO-37 (Pesticide-4)	n.p.	undiluted	2B	2B	III	III	NI	NI	Prinsen (1996)
TNO-38 (Solvent-10)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-39 (Detergent-3)	n.p.	undiluted	NI	NI	IV	IV	NI	NI	Prinsen (1996)
TNO-40 (Glycolbromoacetate form.)	n.p.	undiluted	I	-	I	-	R41	R41 (SC)	Prinsen (1996)
TNO-41 (Amidosulfonic acid)	5329-14-6	undiluted	I	-	I	-	R41	R41 (SC)	Prinsen (1996)
TNO-42 (Glycolbromoacetate)	3785-34-0	85%	I	-	I	-	R41	R41 (SC)	Prinsen (1996)
TNO-43 (Monobromoacetic acid)	79-08-3	undiluted	I	-	I	-	R41	R41 (SC)	Prinsen (1996)
TNO-44 (Didecyldimethylammoniumchloride (23% in propyl glycol))	7173-51-5	23%	I	-	I	-	R41	R41 (SC)	Prinsen (1996)
TNO-45	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-46	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-47	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-48	n.p.	undiluted	2A	-	II	-	R36	R41 (SC)	Prinsen (2005)
TNO-49	n.p.	undiluted	I	-	I	-	R41	R41 (SC)	Prinsen (2005)
TNO-50	n.p.	undiluted	I	-	I	-	R41	R41 (SC)	Prinsen (2005)
TNO-51	n.p.	undiluted	I	-	I	-	R41	R41 (SC)	Prinsen (2005)
TNO-52	n.p.	undiluted	2B	2A	III	III	NI	R36	Prinsen (2005)
TNO-53	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)

**In Vivo and In Vitro Data Comparison  
Sorted by Substance**

Substance/Product Name	CASRN	Concentration Tested	In Vitro Classification (GHS)	In Vivo Classification (GHS)	In Vitro Classification (EPA)	In Vivo Classification (EPA)	In Vitro Classification (EU)	In Vivo Classification (EU)	Reference
TNO-54	n.p.	undiluted	2B	2B	III	III	NI	NI	Prinsen (2005)
TNO-55	n.p.	undiluted	2B	2A	III	III	R36	R36	Prinsen (2005)
TNO-56	n.p.	undiluted	2B	2B	III	III	R36	NI	Prinsen (2005)
TNO-57	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (2005)
TNO-58	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-59	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-60	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-61	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-62	n.p.	undiluted	2B	NI	III	III	R36	NI	Prinsen (2005)
TNO-63	n.p.	undiluted	NI	NI	IV	III	NI	NI	Prinsen (2005)
TNO-64	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (2005)
TNO-65	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-66	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-67	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (2005)
TNO-68	n.p.	undiluted	2A	2A	II	II	R36	R36	Prinsen (2005)
TNO-69	n.p.	50%	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-70	n.p.	undiluted	2A	2A	II	III	R36	R36	Prinsen (2005)
TNO-71	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (2005)
TNO-72	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-73	n.p.	undiluted	I	2A	I	II	R41	R36	Prinsen (2005)
TNO-74	n.p.	undiluted	NI	NI	IV	III	NI	NI	Prinsen (2005)
TNO-75	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-76	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-77	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (2005)
TNO-78	n.p.	undiluted	2B	2B	III	III	NI	NI	Prinsen (2005)
TNO-79	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (2005)
TNO-80	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-81	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-82	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-83	n.p.	undiluted	2B	2B	III	III	NI	R36	Prinsen (2005)
TNO-84	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (2005)
TNO-85	n.p.	undiluted	2B	I	III	I	R36	R41	Prinsen (2005)
TNO-86	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (2005)
TNO-87	n.p.	undiluted	2B	NI	III	IV	NI	NI	Prinsen (2005)
TNO-88	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-89	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-90	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-91	n.p.	undiluted	NI	NI	NI	IV	NI	NI	Prinsen (2005)
TNO-92	n.p.	undiluted	2B	I	III	I	R36	R41	Prinsen (2005)
TNO-93	n.p.	undiluted	2A	I	II	I	R36	R41	Prinsen (2005)
TNO-94	n.p.	undiluted	NI	I	NI	I	NI	R41	Prinsen (2005)
Toluene	108-88-3	undiluted	2A	NI	II	III	R36	NI	Balls et al. (1995)
Triacetin	102-76-1	undiluted	NI	NI	IV	IV	NI	NI	Prinsen and Koëter (1993)

**In Vivo and In Vitro Data Comparison  
Sorted by Substance**

Substance/Product Name	CASRN	Concentration Tested	<i>In Vitro</i> Classification (GHS)	<i>In Vivo</i> Classification (GHS)	<i>In Vitro</i> Classification (EPA)	<i>In Vivo</i> Classification (EPA)	<i>In Vitro</i> Classification (EU)	<i>In Vivo</i> Classification (EU)	Reference
Tributyltin chloride	1461-22-9	undiluted	1	-	I	-	R41	R41	Prinsen and Koëter (1993)
Trichloroacetic acid (3%)	76-03-9	3%	2A	NI	II	III	R36	NI	Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	30%	1	1	I	I	R41	R41	Balls et al. (1995)
Triethanolamine	102-71-6	undiluted	2B	NI	III	III	NI	NI	Prinsen and Koëter (1993)
Triton X-100 (5%)	9002-93-1	5%	2A	2A	II	III	R36	NI	Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	10%	2A/2B	1	II/III	II	R36	R41	Balls et al. (1995)
Triton X-500 (5%)	—	undiluted	2B	-	III	-	NI	R36	Prinsen (2000)
Tween 20	9005-64-5	undiluted	2B	NI	III	III	NI	NI	Balls et al. (1995)

SCNM - Study criteria not met

SC - Classification assigned on the basis of skin corrosion assay

***[This Page Intentionally Left Blank]***

## **Appendix E**

### **Interlaboratory Correlation Coefficients from the EC/HO Validation Study (Balls et al., 1995)**

***[This Page Intentionally Left Blank]***

**Interlaboratory Correlation Coefficients  
from the EC/HO Validation Study (Balls et al., 1995)**

Chemical Category <sup>1</sup>	In Vitro Endpoint	No. samples tested In Vitro	Interlaboratory correlation of <i>in vitro</i> data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
A	BCOPP9	60	a	1.000				
A	BCOPP10	60	b	0.777	1.000			
A	BCOPP11	60	c	0.886	0.862	1.000		
A	BCOPP12	60	d	0.797	0.683	0.859	1.000	
A	BCOPP13	60	e	0.856	0.788	0.906	0.892	1.000
A	BCOPO9	60	a	1.000				
A	BCOPO10	60	b	0.924	1.000			
A	BCOPO11	60	c	0.934	0.898	1.000		
A	BCOPO12	60	d	0.946	0.905	0.978	1.000	
A	BCOPO13	60	e	0.970	0.936	0.953	0.955	1.000
A	BCOPI9	60	a	1.000				
A	BCOPI10	60	b	0.894	1.000			
A	BCOPI11	60	c	0.922	0.896	1.000		
A	BCOPI12	60	d	0.924	0.867	0.957	1.000	
A	BCOPI13	60	e	0.955	0.901	0.947	0.958	1.000
A	BCOPI9b	60	a	1.000				
A	BCOPI10b	60	b	0.898	1.000			
A	BCOPI11b	60	c	0.913	0.913	1.000		
A	BCOPI12b	60	d	0.908	0.848	0.916	1.000	
A	BCOPP13b	60	e	0.939	0.885	0.938	0.938	1.000
A	HETQ14	49	a	1.000				
A	HETQ15	40	b	0.790	1.000			
A	HETQ16	47	c	0.473	0.521	1.000		
A	HETQ17	41	d	0.550	0.734	0.664	1.000	
A	HETS14	11	a	1.000				
A	HETS15	13	b	0.174	1.000			
A	HETS16	13	c	-0.171	-0.171	1.000		
A	HETS17	17	d	-0.103	0.808	0.031	1.000	
A	HETQ14b	49	a	1.000				
A	HETQ15b	40	b	0.627	1.000			
A	HETQ16b	47	c	0.709	0.638	1.000		
A	HETQ17b	41	d	0.449	0.814	0.528	1.000	
A	HETS14b	11	a	1.000				
A	HETS15b	13	b	*	1.000			
A	HETS16b	13	c	-0.043	-0.316	1.000		
A	HETS17b	41	d	*	*	*	*	

**Interlaboratory Correlation Coefficients  
from the EC/HO Validation Study (Balls et al., 1995)**

Chemical Category <sup>1</sup>	In Vitro Endpoint	No. samples tested In Vitro	Interlaboratory correlation of <i>in vitro</i> data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
A	ICES 22	60	a	1.000				
A	ICES 27	60	b	0.721	1.000			
A	ICES 24	59	c	0.750	0.715	1.000		
A	ICES 25	58	d	0.627	0.668	0.734	1.000	
A	ICEO 22	60	a	1.000				
A	ICEO 27	60	b	0.700	1.000			
A	ICEO 24	60	c	0.759	0.716	1.000		
A	ICEO 25	60	d	0.752	0.679	0.732	1.000	
A	ICEF 22	60	a	1.000				
A	ICEF 27	60	b	0.693	1.000			
A	ICEF 24	59	c	0.768	0.525	1.000		
A	ICEF 25	60	d	0.719	0.654	0.690	1.000	
A	ICEC 22	60	a	1.000				
A	ICEC 27	60	b	0.829	1.000			
A	ICEC 24	60	c	0.849	0.759	1.000		
A	ICEC 25	60	d	0.844	0.801	0.853	1.000	
A	IREA 26	60	a	1.000				
A	IREA 23	60	b	0.441	1.000			
A	IREA 28	60	c	0.585	0.695	1.000		
A	IREA 29	60	d	0.619	0.587	0.677	1.000	
A	IREB 26	60	a	1.000				
A	IREB 23	60	b	0.728	1.000			
A	IREB 28	60	c	0.714	0.688	1.000		
A	IREB 29	60	d	0.688	0.617	0.808	1.000	
A	IREC 26	58	a	1.000				
A	IREC 23	60	b	0.524	1.000			
A	IREC 28	58	c	0.485	0.414	1.000		
A	IREC 29	60	d	0.625	0.681	0.819	1.000	
A	IRED 26	58	a	1.000				
A	IRED 23	60	b	0.623	1.000			
A	IRED 28	58	c	0.707	0.618	1.000		
A	IRED 29	60	d	0.813	0.698	0.882	1.000	
A	IRESUM 26	60	a	1.000				
A	IRESUM 23	59	b	0.502	1.000			
A	IRESUM 28	60	c	0.574	0.834	1.000		
A	IRESUM 29	54	d	0.689	0.709	0.798	1.000	



**Interlaboratory Correlation Coefficients  
from the EC/HO Validation Study (Balls et al., 1995)**

Chemical Category <sup>1</sup>	In Vitro Endpoint	No. samples tested In Vitro	Interlaboratory correlation of in vitro data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
B	BCOPP9	30	a	1.000				
B	BCOPP10	30	b	0.733	1.000			
B	BCOPP11	30	c	0.864	0.818	1.000		
B	BCOPP12	30	d	0.760	0.521	0.807	1.000	
B	BCOPP13	30	e	0.880	0.666	0.870	0.840	1.000
B	BCOPO9	30	a	1.000				
B	BCOPO10	30	b	0.945	1.000			
B	BCOPO11	30	c	0.971	0.932	1.000		
B	BCOPO12	30	d	0.962	0.927	0.964	1.000	
B	BCOPO13	30	e	0.959	0.938	0.946	0.928	1.000
B	BCOPI9	30	a	1.000				
B	BCOPI10	30	b	0.906	1.000			
B	BCOPI11	30	c	0.952	0.936	1.000		
B	BCOPI12	30	d	0.929	0.855	0.944	1.000	
B	BCOPI13	30	e	0.950	0.864	0.949	0.948	1.000
B	BCOPI9b	30	a	1.000				
B	BCOPI10b	30	b	0.888	1.000			
B	BCOPI11b	30	c	0.936	0.938	1.000		
B	BCOPI12b	30	d	0.892	0.823	0.916	1.000	
B	BCOPP13b	30	e	0.930	0.850	0.952	0.926	1.000
B	HETQ14	25	a	1.000				
B	HETQ15	17	b	0.711	1.000			
B	HETQ16	23	c	0.355	0.387	1.000		
B	HETQ17	18	d	0.456	0.760	0.679	1.000	
B	HETS14	5	a	*				
B	HETSd15	9	b	*	1.000			
B	HETS16	7	c	*	0.949	1.000		
B	HETS17	11	d	*	0.831	0.420	1.000	
B	HETQ14b	25	a	1.000				
B	HETQ15b	17	b	0.727	1.000			
B	HETQ16b	23	c	0.645	0.594	1.000		
B	HETQ17b	18	d	0.927	0.470	0.535	1.000	
B	ICES 22	30	a	1.000				
B	ICES 27	30	b	0.808	1.000			
B	ICES 24	29	c	0.722	0.789	1.000		
B	ICES 25	29	d	0.691	0.795	0.789	1.000	

**Interlaboratory Correlation Coefficients  
from the EC/HO Validation Study (Balls et al., 1995)**

Chemical Category <sup>1</sup>	In Vitro Endpoint	No. samples tested In Vitro	Interlaboratory correlation of <i>in vitro</i> data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
B	ICEO 22	30	a	1.000				
B	ICEO 27	30	b	0.775	1.000			
B	ICEO 24	30	c	0.775	0.821	1.000		
B	ICEO 25	30	d	0.847	0.812	0.771	1.000	
B	ICEF 22	30	a	1.000				
B	ICEF 27	30	b	0.803	1.000			
B	ICEF 24	29	c	0.846	0.692	1.000		
B	ICEF 25	30	d	0.676	0.727	0.704	1.000	
B	ICEC 22	30	a	1.000				
B	ICEC 27	30	b	0.892	1.000			
B	ICEC 24	30	c	0.881	0.860	1.000		
B	ICEC 25	30	d	0.881	0.896	0.858	1.000	
B	IREA 26	30	a	1.000				
B	IREA 23	30	b	0.503	1.000			
B	IREA 28	30	c	0.624	0.814	1.000		
B	IREA 29	30	d	0.608	0.706	0.701	1.000	
B	IREB 26	30	a	1.000				
B	IREB 23	30	b	0.754	1.000			
B	IREB 28	30	c	0.699	0.746	1.000		
B	IREB 29	30	d	0.690	0.674	0.912	1.000	
B	IREC 26	29	a	1.000				
B	IREC 23	30	b	0.606	1.000			
B	IREC 28	28	c	0.655	0.439	1.000		
B	IREC 29	30	d	0.777	0.733	0.855	1.000	
B	IRED 26	29	a	1.000				
B	IRED 23	30	b	0.663	1.000			
B	IRED 28	28	c	0.799	0.598	1.000		
B	IRED 29	30	d	0.855	0.747	0.939	1.000	
B	IRESUM 26	30	a	1.000				
B	IRESUM 23	29	b	0.568	1.000			
B	IRESUM 28	30	c	0.595	0.955	1.000		
B	IRESUM 29	25	d	0.835	0.749	0.799	1.000	
C	BCOPP9	18	a	1.000				
C	BCOPP10	18	b	0.915	1.000			
C	BCOPP11	18	c	0.932	0.893	1.000		
C	BCOPP12	18	d	0.785	0.688	0.894	1.000	
C	BCOPP13	18	e	0.901	0.889	0.963	0.922	1.000

**Interlaboratory Correlation Coefficients  
from the EC/HO Validation Study (Balls et al., 1995)**

Chemical Category <sup>1</sup>	In Vitro Endpoint	No. samples tested In Vitro	Interlaboratory correlation of <i>in vitro</i> data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
C	BCOPO9	18	a	1.000				
C	BCOPO10	18	b	0.959	1.000			
C	BCOPO11	18	c	0.913	0.896	1.000		
C	BCOPO12	18	d	0.942	0.928	0.991	1.000	
C	BCOPO13	18	e	0.982	0.972	0.961	0.978	1.000
C	BCOPI9	18	a	1.000				
C	BCOPI10	18	b	0.946	1.000			
C	BCOPI11	18	c	0.898	0.879	1.000		
C	BCOPI12	18	d	0.937	0.915	0.980	1.000	
C	BCOPI13	18	e	0.981	0.964	0.947	0.978	1.000
C	BCOPI9b	18	a	1.000				
C	BCOPI10b	18	b	0.943	1.000			
C	BCOPI11b	18	c	0.864	0.877	1.000		
C	BCOPI12b	18	d	0.949	0.916	0.923	1.000	
C	BCOPP13b	18	e	0.971	0.954	0.905	0.968	1.000
C	HETQ14	12	a	1.000				
C	HETQ15	11	b	0.944	1.000			
C	HETQ16	12	c	0.809	0.745	1.000		
C	HETQ17	11	d	0.621	0.580	0.782	1.000	
C	HETS14	6	a	1.000				
C	HETS15	4	b	0.096	1.000			
C	HETS16	6	c	-0.159	-0.910	1.000		
C	HETS17	4	d	-0.288	0.852	-0.094	1.000	
C	HETQ14b	12	a	1.000				
C	HETQ15b	11	b	0.692	1.000			
C	HETQ16b	12	c	0.816	0.642	1.000		
C	HETQ17b	11	d	0.626	0.830	0.562	1.000	
C	ICES 22	18	a	1.000				
C	ICES 27	18	b	0.671	1.000			
C	ICES 24	18	c	0.757	0.599	1.000		
C	ICES 25	17	d	0.514	0.210	0.732	1.000	
C	ICEO 22	18	a	1.000				
C	ICEO 27	18	b	0.498	1.000			
C	ICEO 24	18	c	0.704	0.414	1.000		
C	ICEO 25	18	d	0.786	0.442	0.851	1.000	
C	ICEF 22	18	a	1.000				
C	ICEF 27	18	b	0.433	1.000			
C	ICEF 24	18	c	0.847	0.371	1.000		
C	ICEF 25	18	d	0.745	0.517	0.763	1.000	

**Interlaboratory Correlation Coefficients  
from the EC/HO Validation Study (Balls et al., 1995)**

Chemical Category <sup>1</sup>	In Vitro Endpoint	No. samples tested In Vitro	Interlaboratory correlation of <i>in vitro</i> data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
C	ICEC 22	18	a	1.000				
C	ICEC 27	18	b	0.705	1.000			
C	ICEC 24	18	c	0.844	0.569	1.000		
C	ICEC 25	18	d	0.763	0.595	0.905	1.000	
C	IREA 26	18	a	1.000				
C	IREA 23	18	b	0.413	1.000			
C	IREA 28	18	c	0.599	0.722	1.000		
C	IREA 29	18	d	0.656	0.480	0.634	1.000	
C	IREB 26	18	a	1.000				
C	IREB 23	18	b	0.629	1.000			
C	IREB 28	18	c	0.683	0.552	1.000		
C	IREB 29	18	d	0.607	0.409	0.575	1.000	
C	IREC 26	17	a	1.000				
C	IREC 23	18	b	0.169	1.000			
C	IREC 28	18	c	0.276	0.456	1.000		
C	IREC 29	18	d	0.210	0.392	0.748	1.000	
C	IRED 26	17	a	1.000				
C	IRED 23	18	b	0.490	1.000			
C	IRED 28	18	c	0.704	0.689	1.000		
C	IRED 29	18	d	0.790	0.615	0.874	1.000	
C	IRESUM 26	18	a	1.000				
C	IRESUM 23	18	b	0.481	1.000			
C	IRESUM 28	18	c	0.555	0.861	1.000		
C	IRESUM 29	18	d	0.628	0.964	0.896	1.000	
D	BCOPP9	12	a	1.000				
D	BCOPP10	12	b	0.835	1.000			
D	BCOPP11	12	c	0.932	0.912	1.000		
D	BCOPP12	12	d	0.843	0.966	0.922	1.000	
D	BCOPP13	12	e	0.766	0.924	0.921	0.958	1.000
D	BCOPO9	12	a	1.000				
D	BCOPO10	12	b	0.957	1.000			
D	BCOPO11	12	c	0.971	0.981	1.000		
D	BCOPO12	12	d	0.947	0.972	0.957	1.000	
D	BCOPO13	12	e	0.967	0.995	0.985	0.973	1.000
D	BCOPI9	12	a	1.000				
D	BCOPI10	12	b	0.914	1.000			
D	BCOPI11	12	c	0.951	0.952	1.000		
D	BCOPI12	12	d	0.915	0.989	0.936	1.000	
D	BCOPI13	12	e	0.915	0.959	0.947	0.966	1.000

**Interlaboratory Correlation Coefficients  
from the EC/HO Validation Study (Balls et al., 1995)**

Chemical Category <sup>1</sup>	In Vitro Endpoint	No. samples tested In Vitro	Interlaboratory correlation of <i>in vitro</i> data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
D	BCOPI9b	12	a	1.000				
D	BCOPI10b	12	b	0.914	1.000			
D	BCOPI11b	12	c	0.951	0.952	1.000		
D	BCOPI12b	12	d	0.915	0.989	0.936	1.000	
D	BCOPP13b	12	e	0.915	0.959	0.947	0.966	1.000
D	HETQ14	12	a	1.000				
D	HETQ15	12	b	0.793	1.000			
D	HETQ16	12	c	0.438	0.779	1.000		
D	HETQ17	12	d	0.816	0.876	0.579	1.000	
D	HETQ14b	12	a	1.000				
D	HETQ15b	12	b	0.721	1.000			
D	HETQ16b	12	c	0.670	0.768	1.000		
D	HETQ17b	12	d	0.420	0.966	0.721	1.000	
D	ICES 22	12	a	1.000				
D	ICES 27	12	b	0.741	1.000			
D	ICES 24	12	c	0.920	0.696	1.000		
D	ICES 25	12	d	0.641	0.392	0.543	1.000	
D	ICEO 22	12	a	1.000				
D	ICEO 27	12	b	0.618	1.000			
D	ICEO 24	12	c	0.719	0.759	1.000		
D	ICEO 25	12	d	0.438	0.834	0.483	1.000	
D	ICEF 22	12	a	1.000				
D	ICEF 27	12	b	0.663	1.000			
D	ICEF 24	12	c	0.636	0.546	1.000		
D	ICEF 25	12	d	0.950	0.748	0.664	1.000	
D	ICEC 22	12	a	1.000				
D	ICEC 27	12	b	0.827	1.000			
D	ICEC 24	12	c	0.854	0.805	1.000		
D	ICEC 25	12	d	0.870	0.759	0.724	1.000	
D	IREA 26	12	a	1.000				
D	IREA 23	12	b	0.433	1.000			
D	IREA 28	12	c	0.317	0.567	1.000		
D	IREA 29	12	d	0.678	0.462	0.480	1.000	
D	IREB 26	12	a	1.000				
D	IREB 23	12	b	0.786	1.000			
D	IREB 28	12	c	0.894	0.789	1.000		
D	IREB 29	12	d	0.814	0.736	0.845	1.000	

**Interlaboratory Correlation Coefficients  
from the EC/HO Validation Study (Balls et al., 1995)**

Chemical Category <sup>1</sup>	In Vitro Endpoint	No. samples tested In Vitro	Interlaboratory correlation of <i>in vitro</i> data						
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e	
D	IREC 26	12	a	1.000					
D	IREC 23	12	b	0.091	1.000				
D	IREC 28	12	c	-0.148	0.269	1.000			
D	IREC 29	12	d	-0.010	0.527	0.835	1.000		
D	IREC 26	12	a	1.000					
D	IREC 23	12	b	0.647	1.000				
D	IREC 28	12	c	0.405	0.635	1.000			
D	IREC 29	12	d	0.686	0.589	0.758	1.000		
D	IRESUM 26	12	a	1.000					
D	IRESUM 23	12	b	0.363	1.000				
D	IRESUM 28	12	c	0.769	0.498	1.000			
D	IRESUM 29	11	d	0.665	0.614	0.872	1.000		
E	BCOPP9	20	a	1.000					
E	BCOPP10	20	b	0.773	1.000				
E	BCOPP11	20	c	0.926	0.843	1.000			
E	BCOPP12	20	d	0.878	0.563	0.889	1.000		
E	BCOPP13	20	e	0.932	0.670	0.934	0.886	1.000	
E	BCOPO9	20	a	1.000					
E	BCOPO10	20	b	0.941	1.000				
E	BCOPO11	20	c	0.908	0.887	1.000			
E	BCOPO12	20	d	0.912	0.903	0.977	1.000		
E	BCOPO13	20	e	0.966	0.930	0.952	0.942	1.000	
E	BCOPI9	20	a	1.000					
E	BCOPI10	20	b	0.902	1.000				
E	BCOPI11	20	c	0.897	0.872	1.000			
E	BCOPI12	20	d	0.880	0.852	0.960	1.000		
E	BCOPI13	20	e	0.945	0.884	0.943	0.942	1.000	
E	BCOPI9b	20	a	1.000					
E	BCOPI10b	20	b	0.881	1.000				
E	BCOPI11b	20	c	0.887	0.869	1.000			
E	BCOPI12b	20	d	0.870	0.776	0.889	1.000		
E	BCOPP13b	20	e	0.921	0.824	0.925	0.930	1.000	
E	HETQ14	9	a	1.000					
E	HETQ15	0	b	*	*				
E	HETQ16	7	c	0.500	*	1.000			
E	HETQ17	1	d	*	*	*	*		

**Interlaboratory Correlation Coefficients  
from the EC/HO Validation Study (Balls et al., 1995)**

Chemical Category <sup>1</sup>	In Vitro Endpoint	No. samples tested In Vitro	Interlaboratory correlation of <i>in vitro</i> data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
E	HETS14	11	a	1.000				
E	HETS15	13	b	0.174	1.000			
E	HETS16	13	c	-0.171	-0.171	1.000		
E	HETS17	17	d	-0.103	0.808	0.031	1.000	
E	HETQ14b	9	a	1.000				
E	HETQ15b	0	b	*	*			
E	HETQ16b	7	c	0.985	*	1.000		
E	HETQ17b	1	d	*	*	*	*	
E	ICES 22	20	a	1.000				
E	ICES 27	20	b	0.869	1.000			
E	ICES 24	20	c	0.847	0.734	1.000		
E	ICES 25	19	d	0.778	0.722	0.811	1.000	
E	ICEO 22	20	a	1.000				
E	ICEO 27	20	b	0.595	1.000			
E	ICEO 24	20	c	0.752	0.602	1.000		
E	ICEO 25	20	d	0.868	0.649	0.752	1.000	
E	ICEF 22	20	a	1.000				
E	ICEF 27	20	b	0.729	1.000			
E	ICEF 24	20	c	0.864	0.678	1.000		
E	ICEF 25	20	d	0.739	0.869	0.674	1.000	
E	ICEC 22	20	a	1.000				
E	ICEC 27	20	b	0.806	1.000			
E	ICEC 24	20	c	0.874	0.752	1.000		
E	ICEC 25	20	d	0.883	0.816	0.880	1.000	
E	IREA 26	20	a	1.000				
E	IREA 23	20	b	0.195	1.000			
E	IREA 28	20	c	0.394	0.908	1.000		
E	IREA 29	20	d	0.405	0.543	0.468	1.000	
E	IREB 26	20	a	1.000				
E	IREB 23	20	b	0.782	1.000			
E	IREB 28	20	c	0.629	0.649	1.000		
E	IREB 29	20	d	0.569	0.524	0.672	1.000	
E	IREC 26	19	a	1.000				
E	IREC 23	20	b	0.335	1.000			
E	IREC 28	20	c	0.670	0.404	1.000		
E	IREC 29	20	d	0.559	0.628	0.829	1.000	

**Interlaboratory Correlation Coefficients  
from the EC/HO Validation Study (Balls et al., 1995)**

Chemical Category <sup>1</sup>	In Vitro Endpoint	No. samples tested In Vitro	Interlaboratory correlation of in vitro data						
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e	
E	IREQ 26	19	a	1.000					
E	IREQ 23	20	b	0.540	1.000				
E	IREQ 28	20	c	0.791	0.685	1.000			
E	IREQ 29	20	d	0.798	0.689	0.949	1.000		
E	IRESUM 26	20	a	1.000					
E	IRESUM 23	19	b	0.199	1.000				
E	IRESUM 28	20	c	0.191	0.991	1.000			
E	IRESUM 29	15	d	0.432	0.606	0.635	1.000		
F	BCOPP9	14	a	1.000					
F	BCOPP10	14	b	0.731	1.000				
F	BCOPP11	14	c	0.901	0.864	1.000			
F	BCOPP12	14	d	0.795	0.903	0.896	1.000		
F	BCOPP13	14	e	0.699	0.846	0.875	0.933	1.000	
F	BCOPO9	14	a	1.000					
F	BCOPO10	14	b	0.984	1.000				
F	BCOPO11	14	c	0.985	0.959	1.000			
F	BCOPO12	14	d	0.989	0.968	0.987	1.000		
F	BCOPO13	14	e	0.984	0.988	0.955	0.976	1.000	
F	BCOPI9	14	a	1.000					
F	BCOPI10	14	b	0.917	1.000				
F	BCOPI11	14	c	0.975	0.920	1.000			
F	BCOPI12	14	d	0.974	0.914	0.974	1.000		
F	BCOPI13	14	e	0.969	0.926	0.954	0.980	1.000	
F	BCOPI9b	14	a	1.000					
F	BCOPI10b	14	b	0.899	1.000				
F	BCOPI11b	14	c	0.970	0.928	1.000			
F	BCOPI12b	14	d	0.955	0.921	0.962	1.000		
F	BCOPP13b	14	e	0.946	0.918	0.976	0.972	1.000	
F	HETQ14	14	a	1.000					
F	HETQ15	14	b	0.880	1.000				
F	HETQ16	14	c	0.776	0.730	1.000			
F	HETQ17	14	d	0.712	0.842	0.765	1.000		
F	HETQ14b	14	a	*					
F	HETQ15b	14	b	*	1.000				
F	HETQ16b	14	c	*	0.591	1.000			
F	HETQ17b	14	d	*	0.974	0.590	1.000		



**Interlaboratory Correlation Coefficients  
from the EC/HO Validation Study (Balls et al., 1995)**

Chemical Category <sup>1</sup>	In Vitro Endpoint	No. samples tested In Vitro	Interlaboratory correlation of <i>in vitro</i> data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
F	ICES 22	14	a	1.000				
F	ICES 27	14	b	0.617	1.000			
F	ICES 24	13	c	0.757	0.856	1.000		
F	ICES 25	13	d	0.539	0.889	0.821	1.000	
F	ICEO 22	14	a	1.000				
F	ICEO 27	14	b	0.797	1.000			
F	ICEO 24	14	c	0.796	0.907	1.000		
F	ICEO 25	14	d	0.794	0.868	0.717	1.000	
F	ICEF 22	14	a	1.000				
F	ICEF 27	14	b	0.781	1.000			
F	ICEF 24	13	c	0.604	0.543	1.000		
F	ICEF 25	14	d	0.901	0.689	0.772	1.000	
F	ICEC 22	14	a	1.000				
F	ICEC 27	14	b	0.873	1.000			
F	ICEC 24	14	c	0.877	0.905	1.000		
F	ICEC 25	14	d	0.907	0.913	0.868	1.000	
F	IREA 26	14	a	1.000				
F	IREA 23	14	b	0.648	1.000			
F	IREA 28	14	c	0.733	0.712	1.000		
F	IREA 29	14	d	0.789	0.596	0.817	1.000	
F	IREB 26	14	a	1.000				
F	IREB 23	14	b	0.808	1.000			
F	IREB 28	14	c	0.862	0.812	1.000		
F	IREB 29	14	d	0.789	0.746	0.906	1.000	
F	IREC 26	13	a	1.000				
F	IREC 23	14	b	0.914	1.000			
F	IREC 28	12	c	0.464	0.682	1.000		
F	IREC 29	14	d	0.805	0.815	0.845	1.000	
F	IRED 26	13	a	1.000				
F	IRED 23	14	b	0.776	1.000			
F	IRED 28	12	c	0.613	0.575	1.000		
F	IRED 29	14	d	0.868	0.696	0.781	1.000	
F	IRESUM 26	14	a	1.000				
F	IRESUM 23	14	b	0.770	1.000			
F	IRESUM 28	14	c	0.863	0.811	1.000		
F	IRESUM 29	14	d	0.884	0.800	0.957	1.000	

**Interlaboratory Correlation Coefficients  
from the EC/HO Validation Study (Balls et al., 1995)**

Chemical Category <sup>1</sup>	In Vitro Endpoint	No. samples tested In Vitro	Interlaboratory correlation of <i>in vitro</i> data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
G	BCOPP9	26	a	1.000				
G	BCOPP10	26	b	0.733	1.000			
G	BCOPP11	26	c	0.801	0.856	1.000		
G	BCOPP12	26	d	0.781	0.612	0.801	1.000	
G	BCOPP13	26	e	0.893	0.794	0.858	0.845	1.000
G	BCOPO9	26	a	1.000				
G	BCOPO10	26	b	0.961	1.000			
G	BCOPO11	26	c	0.935	0.955	1.000		
G	BCOPO12	26	d	0.949	0.961	0.967	1.000	
G	BCOPO13	26	e	0.961	0.964	0.913	0.940	1.000
G	BCOPI9	26	a	1.000				
G	BCOPI10	26	b	0.873	1.000			
G	BCOPI11	26	c	0.875	0.939	1.000		
G	BCOPI12	26	d	0.897	0.851	0.902	1.000	
G	BCOPI13	26	e	0.953	0.891	0.898	0.956	1.000
G	BCOPI9b	26	a	1.000				
G	BCOPI10b	26	b	0.873	1.000			
G	BCOPI11b	26	c	0.875	0.939	1.000		
G	BCOPI12b	26	d	0.897	0.851	0.902	1.000	
G	BCOPP13b	26	e	0.953	0.891	0.898	0.956	1.000
G	HETQ14	26	a	1.000				
G	HETQ15	26	b	0.755	1.000			
G	HETQ16	26	c	0.221	0.450	1.000		
G	HETQ17	26	d	0.492	0.692	0.704	1.000	
G	HETQ14b	26	a	1.000				
G	HETQ15b	26	b	0.721	1.000			
G	HETQ16b	26	c	0.771	0.638	1.000		
G	HETQ17b	26	d	0.675	0.765	0.591	1.000	
G	ICES 22	26	a	1.000				
G	ICES 27	26	b	0.779	1.000			
G	ICES 24	26	c	0.690	0.736	1.000		
G	ICES 25	26	d	0.626	0.461	0.560	1.000	
G	ICEO 22	26	a	1.000				
G	ICEO 27	26	b	0.757	1.000			
G	ICEO 24	26	c	0.770	0.695	1.000		
G	ICEO 25	26	d	0.719	0.692	0.764	1.000	

**Interlaboratory Correlation Coefficients  
from the EC/HO Validation Study (Balls et al., 1995)**

Chemical Category <sup>1</sup>	In Vitro Endpoint	No. samples tested In Vitro	Interlaboratory correlation of in vitro data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
G	ICEF 22	26	a	1.000				
G	ICEF 27	26	b	0.607	1.000			
G	ICEF 24	26	c	0.748	0.394	1.000		
G	ICEF 25	26	d	0.594	0.494	0.654	1.000	
G	ICEC 22	26	a	1.000				
G	ICEC 27	26	b	0.856	1.000			
G	ICEC 24	26	c	0.830	0.745	1.000		
G	ICEC 25	26	d	0.778	0.751	0.803	1.000	
G	IREA 26	26	a	1.000				
G	IREA 23	26	b	0.496	1.000			
G	IREA 28	26	c	0.685	0.518	1.000		
G	IREA 29	26	d	0.709	0.625	0.704	1.000	
G	IREB 26	26	a	1.000				
G	IREB 23	26	b	0.525	1.000			
G	IREB 28	26	c	0.628	0.526	1.000		
G	IREB 29	26	d	0.664	0.470	0.824	1.000	
G	IREC 26	26	a	1.000				
G	IREC 23	26	b	0.137	1.000			
G	IREC 28	26	c	0.245	0.214	1.000		
G	IREC 29	26	d	0.342	0.101	0.808	1.000	
G	IRED 26	26	a	1.000				
G	IRED 23	26	b	0.539	1.000			
G	IRED 28	26	c	0.712	0.507	1.000		
G	IRED 29	26	d	0.790	0.613	0.906	1.000	
G	IRESUM 26	26	a	1.000				
G	IRESUM 23	26	b	0.527	1.000			
G	IRESUM 28	26	c	0.693	0.793	1.000		
G	IRESUM 29	25	d	0.626	0.696	0.716	1.000	

Abbreviations: BCOPI = Index; BCOPIb = Index, cut-off at 200; BCOPO = Opacity; BCOPP = Permeability; ICEC = Irritation Index; ICEF = Fluorescein retention; ICEO = Opacity; ICES = Swelling; IREA = Opacity (1 hr); IREB = Opacity (4 hr); IREC = Swelling (1 hr); IRED = Swelling (4 hr); IRESUM = Summary score; HETQ = Q Score; HETQB = Q Score, cutoff at 2; HETS = S Score; HETSB = S Score, cutoff at 2.

<sup>1</sup>A = Full set of chemicals; B= Water soluble; C = Water insoluble; D = Surfactants; E = Solids; F = Solutions; G = Liquids

The numbers 1-38 against each endpoint in the Table refer to the laboratories which conducted each particular test. Laboratory 36 left the study without submitting any results

\* = No data

***[This Page Intentionally Left Blank]***