

Annex II

Physicochemical Properties of Substances Evaluated in the rLLNA

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Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
(16-beta)-21-(Acetyloxy)-17-hydroxy-16-methylpregna-1,4,9(11)-triene-3,20-dione	17,21-Dihydroxy-16beta-methylpregna-1,4,9(11)-triene-3,20-dione 21-acetate	910-99-6	398.50	3.56	Solid	Pharmaceutical chemicals	GSK
(1r)-1,2,3,4-Tetrahydro-6,7-dimethoxy-2-methyl-1-[(3,4,5-trimethoxyphenyl)methyl]isoquinoline [r-(r*,r*)]-2,3-bis(benzoyloxy)-butanedioate (1:1)	–	104832-01-1	745.79	3.16	Solid	Pharmaceutical chemicals	GSK
(1R,4R)-4-Isopropenyl-1-methyl-2-methylenecyclohexane	–	–	–	–	–	–	LLNA/EC3 Validation Study
(2-Bromo-5-propoxyphenyl)(2-hydroxy-4-methoxyphenyl)-methadone	–	190965-45-8	365.23	5.26	Solid	Pharmaceutical chemicals	GSK
(2e)-2-[(2-Formyl-4-hydroxyphenyl)-methylidene]-butanedioic acid	–	773059-57-7	250.21	0.83	Solid	Pharmaceutical chemicals	GSK
(2-Oxo-1-phenyl-pyrrolidin-3-yl)(triphenyl)-phosphonium bromide	–	148776-18-5	502.40	7.51	Solid	Pharmaceutical chemicals	GSK
(2R,4S)-4-(4-Acetyl-1-piperazinyl)-n-[(1r)-1-[3,5-bis(trifluoro-methyl)phenyl]ethyl]-2-(4-fluoro-2-methylphenyl)-n-methyl-1-piperidine-carboxamide monomethane-sulfonate	–	414910-30-8	712.73	5.63	Solid	Pharmaceutical chemicals	GSK
(2S,4S)-1-[(2s)-2-Amino-3,3-bis(4-fluorophenyl)-1-oxopropyl]-4-fluoro-2-pyrrolidine carbonitrile	Denagliptin	483369-58-0	373.38	2.31	Solid	Pharmaceutical chemicals	GSK

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
(3as,4r,5s,6s,8r,9r,9ar,10r)-6-Ethenyldeca-hydro-5-hydroxy-4,6,9,10-tetramethyl-1-oxo-3a,9-propano-3ah-cyclopentacyclo-octen-8-yl [[[3-exo)-8-methyl-8-azabicyclo-[3.2.1]oct-3-yl]thio]-acetate	Retapamulin	224452-66-8	517.78	5.21	Solid	Pharmaceutical chemicals	GSK
(3as,4r,5s,6s,8r,9r,9ar,10r)-6-Ethenyldeca-hydro-5-hydroxy-4,6,9,10-tetra-methyl-1-oxo-3a,9-propano-3ah-cyclopentacycloocten-8-yl hydroxyacetate	Pleuromulin	125-65-5	378.51	3.98	Solid	Pharmaceutical chemicals	GSK
(3-Endo)-8-methyl-8-azabicyclo[3.2.1]-octan-3-ol	Tropine	120-29-6	141.22	-0.39	Solid	Pharmaceutical chemicals	GSK
(3r,3as,6ar)-Hexahydrofuro-[2,3-b]furan-3-ol	–	156928-09-5	130.14	-1.19	Solid	Pharmaceutical chemicals	GSK
(3r,3as,6ar)-Hexahydrofuro-[2,3-b]furan-3-yl [(1s,2r)-3-[(1,3-benzodioxol-5-ylsulfonyl)(2-methylpropyl)-amino]-2-hydroxy-1-[[4-[(2-methyl-4-thiazolyl)methoxy]phenyl]methyl]-propyl]carbamate	Brecanavir	313682-08-5	703.84	4.32	Solid	Pharmaceutical chemicals	GSK
(3R6R)-3-(2,3-Dihydro-1h-inden-2-yl)-1-[(1r)-1-(2-methyl-1,3-oxazol-4-yl)-2-(4-morpholinyl)-2-oxoethyl]-6-[(1s)-1-methylpropyl]-2,5-piperazinedione	–	820957-38-8	494.60	2.89	Solid	Pharmaceutical chemicals	GSK

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
(3S,6R)-3-isopropyl-6-methylcyclohexene	(+)-trans-p-Menth-2-ene	5113-93-9	138.25	4.70	Liquid	–	LLNA/EC3 Validation Study
(4r,5s)-(-)-1,5-Dimethyl-4-phenyl-2-imidazolidinone	–	92841-65-1	190.25	1.38	Solid	Pharmaceutical chemicals	GSK
(4r,5s)-1,5-Dimethyl-3-(1-oxo-2-propenyl)-4-phenyl-2-imidazolidinone	–	139109-23-2	244.30	3.33	Solid	Pharmaceutical chemicals	GSK
(4S)-1-(tert-Butoxycarbonyl)-4-fluoro-L-prolinamide	–	426844-22-6	232.26	0.98	Solid	Pharmaceutical chemicals	GSK
(4S)-1-(tert-Butoxycarbonyl)-4-fluoro-L-proline	–	203866-13-1	233.24	1.75	Solid	Pharmaceutical chemicals	GSK
(4S,5R)-1-[(1R,2R,3S)-3-(1,3-Benzodioxol-5-yl)-1-(2-benzyloxy-4-methoxyphenyl)-1-hydroxy-6-propoxy-2-indanoyl]-3,4-dimethyl-5-phenyl-2-imidazolidinone	–	190965-47-0	740.86	9.58	Solid	Pharmaceutical chemicals	GSK
(4Z)-2-Methyl-6-methyleneoct-4-ene	–	–	–	–	–	–	LLNA/EC3 Validation Study
(5R)-5-Isopropenyl-2-methyl-1-methylene-2-cyclohexene	–	–	–	–	Liquid	–	LLNA/EC3 Validation Study
(Alpha-r)-n-alpha-dimethyl-3,5-bis(trifluoro-methyl	–	334477-60-0	409.30	3.59	Solid	Pharmaceutical chemicals	GSK
(R,S)-3-Amino-2,3,4,5-tetrahydro-n-(1-methylethyl)-2,4-dioxo-n,5-diphenyl-1h-1,5-benzodiazepine-1-acetamide	–	184944-86-3	442.52	3.21	Solid	Pharmaceutical chemicals	GSK
(s)-(-)-1-Phenylpropyl-amine	–	3789-59-1	135.21	1.93	Liquid	Pharmaceutical chemicals	GSK

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
(S)-2-(4-Fluoro-2-methylphenyl)4-piperidinone (s)-alpha-hydroxybenzene-acetic acid salt	–	414910-13-7	359.40	1.68	Solid	Pharmaceutical chemicals	GSK
[3aS-(3aAlpha,4beta,5alpha,6alpha,8beta,9alpha,9abeta,10S*)]-6-Ethenyldecahydro-5-hydroxy-4,6,9,10-tetramethyl-1-oxo-3a,9-propano-3aH-cyclopentacycloocten-8-yl [(methylsulfonyl)-oxy]acetate	–	60924-38-1	456.60	4.11	Solid	Pharmaceutical chemicals	GSK
[4-(Ethoxymethyl)-2,6-dimethoxyphenyl]-boronic acid	–	591249-50-2	240.07	1.79	Solid	Pharmaceutical chemicals	GSK
[4S-[1(E),4A]alpha,5alpha]-1-[3-[2-[4-Methoxy-2-(phenylmethoxy)-benzoyl]-4-propoxyphenyl]-1-oxo-2-propenyl]-3,4-dimethyl-5-phenyl-2-imidazoli-dinone	–	190965-46-9	618.74	9.34	Solid	Pharmaceutical chemicals	GSK
1-(2',3',4',5'-Tetramethylphenyl)-3-(4'-tetrabutylphenyl)-propane-1,3-dione	–	–	336.47	5.35	–	–	Gerberick
1-(2',3',4',5'-Tetramethylphenyl)butane-1,3-dione	–	167998-73-4	221.32	3.14	–	–	Gerberick
1-(2,3-epoxypropoxy)-2,2-bis[(2,3-epoxypropoxy)methyl]butane	–	–	–	–	–	–	BGIA
1-(2',5' Dimethylphenyl)butane-1,3-dione	–	56290-55-2	193.27	2.65	–	–	Gerberick
1-(2',5'-diethylphenyl)butane-1,3-dione	–	167998-76-7	221.32	3.14	–	–	Gerberick

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
1-(3',4',5'-Tetramethoxyphenyl)-4-dimethylpentane-1,3-dione	–	135099-98-8	297.37	2.47	–	–	Gerberick
1-(4-Ethoxy-phenyl)-2-[4-(methyl-sulfonyl)phenyl]-ethanone	–	346413-00-1	318.40	2.46	Solid	Pharmaceutical chemicals	GSK
1-(p-methoxyphenyl)-1-penten-3-one	Powdery ketone	104-27-8	190.24	2.65	Solid	–	Gerberick
1,1,3-Trimethyl-2-formylcyclohexa-2,4-dione	Safranal	116-26-7	150.22	2.54	Liquid	Hydrocarbons, Cyclic	Gerberick
1,1-Dimethylethyl [(1s)-1-[bis(4-fluorophenyl)-methyl]-2-[(2s,4s)-2-cyano-4-fluoro-1-pyrrolidinyl]-2-oxoethyl]carbamate	–	483368-24-7	473.50	4.14	Solid	Pharmaceutical chemicals	GSK
1,1-Dimethylethyl [(1s)-2-[4-[(2-methyl-4-thiazolyl)methoxy]phenyl]-1-(2s)-oxiranylethyl]-carbamate	–	313680-92-1	390.51	3.32	Solid	Pharmaceutical chemicals	GSK
1,1-Dimethylethyl 3-[[[(3s)-2,3,4,5-tetrahydro-1-[2-[(1-methylethyl)phenylamino]-2-oxoethyl]-2,4-dioxo-5-phenyl-1h-1,5-benzodiazepin-3-yl]amino]carbonyl]amino]benzoate	–	305366-94-3	661.76	6.74	Solid	Pharmaceutical chemicals	GSK
1,2,3,5,6,7-Hexahydro-2-thioxo-4h-cyclopentapyrimidin-4-one	–	35563-27-0	168.22	0.65	Solid	Pharmaceutical chemicals	GSK
1,2-Benzisothiazolin-3-one	Proxan; Proxel active	2634-33-5	151.19	1.42	Solid	Sulfur Compounds; Heterocyclic Compounds	Gerberick

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
1,2-Diaminocyclohexane	cis-1,2-Cyclohexanediamine	1436-59-5	114.19	0.09	Liquid	Amines	BGIA
1,2-Dibromo-2,4-dicyanobutane	–	35691-65-7	265.93	1.91	Solid	Nitriles	Gerberick
1,3-Benzodioxazole-5-sulphonyl chloride	–	115010-10-1	220.63	0.14	Solid	Pharmaceutical chemicals	GSK
1,4-dihydroquinone	–	123-31-9	110.11	1.17	Solid	Phenols	Gerberick
1,6-Bis(2,3-epoxypropoxy)hexane	Diglycidyl hexanediol; 1,6-Hexanediol diglycidyl ether	16096-31-4	230.30	0.84	Liquid	Ethers	BGIA
1-[3-(Cyclopentyl-oxy)-4-methoxy-phenyl]-4-oxocyclohexane carbonitrile	–	152630-47-2	313.40	2.23	Solid	Pharmaceutical chemicals	GSK
1-[5-[(4-Fluorophenyl)methyl]-2-furanyl]ethanone	–	280571-34-8	218.23	2.97	Solid	Pharmaceutical chemicals	GSK
12-Bromo-1-dodecanol	12-Bromolauryl alcohol	3344-77-2	265.23	3.40	Solid	Alcohols	Gerberick
12-Bromododecanoic acid	12-Bromolauric acid	73367-80-3	279.21	3.02	Solid	Lipids	Gerberick
14-Hydroxynor-morphinone	–	84116-46-1	285.30	NA	Solid	Pharmaceutical chemicals	GSK
1-Bromobutane	–	109-65-9	137.02	1.82	Liquid	Hydrocarbons, Halogenated	Gerberick
1-Bromodocosane	–	6938-66-5	389.51	6.25	Solid	Hydrocarbons, Halogenated	Gerberick
1-Bromododecane	Lauryl bromide	143-15-7	249.23	3.79	Liquid	Hydrocarbons, Halogenated	Gerberick
1-Bromoeicosane	–	4276-49-7	361.45	5.76	Solid	Hydrocarbons, Halogenated	Gerberick

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1-Bromoheptadecane	–	3508-00-7	319.36	5.02	Solid	Hydrocarbons, Halogenated	Gerberick
1-Bromohexadecane	n-Hexadecyl bromide; Palmityl bromide; Cetyl bromide	112-82-3	305.34	4.77	Liquid	Hydrocarbons, Halogenated	Gerberick
1-Bromohexane	n-Hexyl bromide	111-25-1	165.07	2.31	Liquid	Hydrocarbons, Halogenated	Gerberick
1-Bromononane	–	693-58-3	207.15	3.05	Liquid	Hydrocarbons, Halogenated	Gerberick
1-Bromooctadecane	–	112-89-0	333.39	5.26	Liquid	Hydrocarbons, Halogenated	Gerberick
1-Bromopentadecane	n-Pentadecyl bromide	629-72-1	291.31	4.53	Liquid	Hydrocarbons, Halogenated	Gerberick
1-Bromotetradecane	–	112-71-0	277.28	4.28	Liquid	Hydrocarbons, Halogenated	Gerberick
1-Bromotridecane	–	765-09-3	263.26	4.03	Liquid	Hydrocarbons, Halogenated	Gerberick
1-Bromoundecane	–	693-67-4	235.20	3.54	Liquid	Hydrocarbons, Halogenated	Gerberick
1-Butanol	–	71-36-3	74.12	1.06	Liquid	Alcohols; Lipids	Gerberick
1-Chloro-2-dinitrobenzene	Dinitrochlorobenzene	97-00-7	202.55	-0.06	Solid	Hydrocarbon, Halogenated; Nitro Compounds; Hydrocarbons, Cyclic	NTP, Gerberick
1-Chlorohexadecane	–	4860-03-1	260.89	4.65	Liquid	Hydrocarbons, Halogenated	Gerberick

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
1-Chloromethylpyrene	–	1086-00-6	250.72	4.89	Solid	Hydrocarbons, Cyclic; Polycyclic Compounds	Gerberick
1-Chlorononane	n-Nonyl chloride	2473-01-0	162.70	2.93	Liquid	Hydrocarbons, Halogenated	Gerberick
1-Chlorooctadecane	Stearyl chloride	3386-33-2	288.94	5.14	Liquid	Hydrocarbons, Halogenated	Gerberick
1-Chlorotetradecane	Myristyl chloride	2425-54-9	232.83	4.16	Liquid	Hydrocarbons, Halogenated	Gerberick
1-Iododecane	–	4292-19-7	296.24	3.91	Liquid	Hydrocarbons, Halogenated	Gerberick
1-Iodohexadecane	Palmityl iodide; Hexadecyl iodide	544-77-4	352.34	4.89	Liquid/Solid	Hydrocarbons, Halogenated	Gerberick
1-Iodohexane	–	638-45-9	212.07	2.43	Liquid	Hydrocarbons, Halogenated	Gerberick
1-Iodononane	n-Nonyl iodide	4282-42-2	254.15	3.17	Liquid	Hydrocarbons, Halogenated	Gerberick
1-Iodooctadecane	–	629-93-6	380.39	5.39	Solid	Hydrocarbons, Halogenated	Gerberick
1-Iodotetradecane	Myristyl iodide, n-Tetradecyl iodide	19218-94-1	324.29	4.40	–	Hydrocarbons, Halogenated	Gerberick
1-Methyl-3-nitronitrosoguanidine	MNNG	70-25-7	147.09	-2.13	Solid	Amidines; Nitroso Compounds	Gerberick
1-Napthol	–	90-15-3	144.17	2.54	Solid	Hydrocarbons, Cyclic	Gerberick
1-Phenyl-1,2-propanedione	–	579-07-7	148.16	1.91	Liquid	Ketones; Heterocyclic Compounds	Gerberick

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1-Phenyl-2-methylbutane-1,3-dione	–	6668-24-2	179.24	2.40	–	–	Gerberick
1-Phenyloctane-1,3-dione	–	55846-68-1	221.32	3.14	–	–	Gerberick
2-(3,4-Dimethyl-phenyl)-5-methyl-2,4-dihydropyrazol-3-one	–	18048-64-1	202.26	2.28	Solid	Pharmaceutical chemicals	GSK
2-(4-Amino-2nitro-phenylamino)-ethanol	HC Red No. 3	2871-01-4	197.19	0.12	Solid	Amines	Gerberick
2-(4-Ethoxyphenyl)-3-[4-(methyl-sulfonyl)phenyl]pyrazolo[1,5-b]-pyridazine	GW 406381	221148-46-5	393.47	3.86	Solid	Pharmaceutical chemicals	GSK
2-(4-Oxopentyl)-1h-isoindole-1,3(2h)-dione	–	3197-25-9	231.25	1.57	Solid	Pharmaceutical chemicals	GSK
2-(4-tert-Amylcyclohexyl) acetaldehyde	QRM 2113	620159-84-4	196.33	3.28	–	–	Gerberick
2-(Benzyl)tert-butylamino)-1-(alpha,4-dihydroxy-m-tolyl)ethane	alpha-((Benzyl-tert-butylamino)methyl)-m-xylene-4,alpha,alpha'-triol	24085-03-8	329.44	2.51	Solid	Pharmaceutical chemicals	GSK
2,2,6,6-Tetramethyl-heptane-3,5-dione	–	1118-71-4	186.30	2.40	Liquid	Ketones	Gerberick
2,2-bis-[4-(2-hydroxy-3 methacryloxypropoxy)phenyl]-propane	Bis-GMA	1565-94-2	512.59	4.94	Liquid	Carboxylic Acids; Phenols; Macromolecular Substances	LLNA/EC3 Validation Study
2,3,4,5-Tetrahydro-n-(1-methylethyl)-2,4-dioxo-n,5-diphenyl-3-[(phenylmethoxy)-imino]-1h-1,5-benzodiazepine-1-acetamide	–	305366-97-6	546.63	7.64	Solid	Pharmaceutical chemicals	GSK
2,3-Butanedione	Erythritol anhydride; Butadiene diepoxide	431-03-8	86.09	0.68	Liquid	Ketones	Gerberick

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
2,3-Dimethyl-2h-indazol-6-amine	–	444731-72-0	161.21	1.01	Solid	Pharmaceutical chemicals	GSK
2,4,6-Trichloro-1,3,5-triazine	Cyanuric chloride	108-77-0	184.41	0.78	Solid	Heterocyclic Compounds	Gerberick
2,4-Diaminophenoxyethanol HCl	–	66422-95-5	168.19	-1.28	–	Amines	LLNA/EC3 Validation Study
2,4-Dichloro-pyrimidine	–	3934-20-1	148.98	1.17	Solid	Pharmaceutical chemicals	GSK
2,4-Heptadienal	–	5910-85-0	110.16	1.80	–	Aldehydes; Hydrocarbons, Acyclic	Gerberick
2,4-Hexadienal	–	142-83-6	96.13	1.37	Liquid	Aldehydes; Hydrocarbons, Acyclic	LLNA/EC3 Validation Study
2,5-Diaminotoluene	–	95-70-5	122.08 (sulfate 156.25)	1.42	Solid (sulfate)	Amines	Gerberick
2,6-Dimethoxy-4-methyl-5-[3-(trifluoromethyl)-phenoxy]-8-quinolinamine	–	106635-86-3	378.35	5.73	Solid	Pharmaceutical chemicals	GSK
2,6-Dimethoxy-4-methyl-8-nitro-5-[3-(trifluoromethyl)-phenoxy]quinoline	–	189746-15-4	408.34	6.09	Solid	Pharmaceutical chemicals	GSK
2,4-Dinitrobenzene sulfonic acid	DNBS	89-02-1	248.17	-1.53	Liquid	Hydrocarbons, Cyclic; Sulfur Compounds	Ryan
2-[(Benzyloxy)-imino]malonic acid	–	305366-96-5	223.19	1.36	Solid	Pharmaceutical chemicals	GSK

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2-[1-(4-Bromophenyl)-1-phenylethoxy]-n,n-dimethylethanamine hydrochloride	Bromadryl	13977-28-1	384.75	4.71	Solid	Pharmaceutical chemicals	GSK
2-Acetylcyclohexanone	–	874-23-7	143.21	1.66	Solid	Hydrocarbons, Cyclic; Ketones	Gerberick
2-Amino-6-chloro-4-nitrophenol	–	6358-09-4	188.57	0.26	Solid	Amines	Gerberick
2-Amino-di-phenylamine	–	534-85-0	184.24	2.39	Solid	Pharmaceutical chemicals	GSK
2-Aminoethyl-methylsulfone	–	49773-20-8	159.63	-1.64	Solid	Pharmaceutical chemicals	GSK
2-Aminophenol	o-Aminophenol; 2-Hydroxyaniline	95-55-6	109.13	1.17	Solid	Amines; Phenols	Gerberick
2-Benzyl-tert-butylamino-3'-hydroxymethyl-4'-hydroxyaceto-phenone hydrochloride	Ethanone, 2-((1,1-dimethylethyl)(phenylmethyl)amino)-1-(4-hydroxy-3-(hydroxymethyl)phenyl)-, hydrochloride	24085-08-3	363.89	3.34	Solid	Pharmaceutical chemicals	GSK
2-Bromo-5-hydroxy-benzaldehyde	–	2973-80-0	201.02	2.45	Solid	Pharmaceutical chemicals	GSK
2-Bromo-5-propoxybenzoic acid	–	190965-43-6	259.10	3.33	Solid	Pharmaceutical chemicals	GSK
2-Bromotetradecanoic acid	2-Bromomyristic acid	10520-81-7	307.27	3.51	Solid	Carboxylic Acids	Gerberick
2-Chloro-6-methoxy-4-methylquinoline	–	6340-55-2	207.66	3.57	Solid	Pharmaceutical chemicals	GSK
2-Hydroxyethyl acrylate	HEA	818-61-1	116.12	0.54	Liquid	Carboxylic Acids	Gerberick
2-Hydroxypropyl methacrylate	2-HPMA	923-26-2	144.17	1.03	Solid	Carboxylic Acids	Gerberick

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2-Mercaptobenzothiazole	Captax	149-30-4	167.25	1.80	Solid	Heterocyclic Compounds	Gerberick
2-Methoxy-4-methylphenol	Cresol	93-51-6	138.16	1.66	Liquid	Phenols	Gerberick
2-Methyl-2H-isothiazol-3-one	–	2682-20-4	115.15	0.68	Solid	Sulfur Compounds; Heterocyclic Compounds	Gerberick
2-Methyl-4H,3,1-benzoxazin-4-one	Product 240	525-76-8	161.16	1.52	Solid	–	Gerberick
2-Methyl-5-hydroxyethylaminophenol	–	55302-96-0	167.21	1.32	–	–	Gerberick
2-Methylundecanal	–	110-41-8	184.32	3.03	Liquid	Aldehydes	Gerberick
2-Morpholinoethyl isocyanide	–	443882-99-3	281.67	4.55	Solid	Pharmaceutical chemicals	GSK
2-Nitro-4-(propylthio)benzenamine	–	54393-89-4	212.27	3.45	Liquid	Pharmaceutical chemicals	GSK
2-Nitro-p-phenylenediamine	–	5307-14-2	153.13	0.01	Solid	Amines	Gerberick
3 and 4-(4-Hydroxy-4-methylpentyl)-3-cyclohexane-1-carboxaldehyde	Lyril	31906-04-4	210.32	2.89	Liquid	Aldehydes; Hydrocarbons, Cyclic	Gerberick
3, 3', 4', 5-Tetrachlorosalicylanilide	3,5-Dichloro-N-(3,4-dichlorophenyl)-2-hydroxybenzamide; TCS	1154-59-2	351.01	3.49	Solid	Amides; Amines	Gerberick
3,4-Dichloroaniline hydrochloride	–	95-76-1	162.02	2.60	Solid	Pharmaceutical chemicals	GSK
3,4-Dihydrocoumarin	Hydroxydihydro-cinnamic acid lactone	119-84-6	148.16	1.91	Liquid	Heterocyclic Compounds	Gerberick
3,4-epoxycyclohexylethyl-cyclopolymethylsiloxane	Tet-sil	–	–	–	–	–	LLNA/EC3 Validation Study

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
3,5,5-Trimethylhexanoyl chloride	–	36727-29-4	176.68	2.54	Liquid	Carboxylic Acids	Gerberick
3-[(2r)-3-[[2-(2,3-Dihydro-1h-inden-2-yl)-1,1-dimethyl-ethyl]amino]-2-hydroxypropoxy]-4,5-difluorobenzene propanoic acid	–	753449-67-1	447.53	2.13	Solid	Pharmaceutical chemicals	GSK
3'-[(2z)-[1-(3,4-Dimethylphenyl)-1,5-dihydro-3-methyl)-5-oxo-4h-pyrazol-4-ylidene]hydrazino]-2'-hydroxy-[1,1'-biphenyl]-3-carboxylic acid, compound with 2-aminoethanol (2:1)	Eltrombopag Olamine	496775-62-3	564.65	5.25	Solid	Pharmaceutical chemicals	GSK
3-[4-[(6-Bromohexyl)oxy]-butyl]benzene-sulfonamide	–	452342-04-0	392.36	3.48	Solid	Pharmaceutical chemicals	GSK
3-Aminomethyl-3,5,5-trimethylcyclohexylamine	5-Amino-1,3,3-trimethylcyclohexanemethylamine; IPDA; Isophorone diamine	2855-13-2	170.30	1.90	Liquid	Amines	BGIA
3-Aminophenol	m-Aminophenol; 3-Hydroxyaniline	591-27-5	109.13	1.17	Solid	Amines; Phenols	Gerberick
3-Bromomethyl-5, 5'-dimethyl-dihydro-2(3H)-furanone	–	154750-20-6	207.07	1.79	–	–	Gerberick
3-Chloro-4-fluorobenzoyl chloride	–	65055-17-6	193.01	2.42	Solid	Pharmaceutical chemicals	GSK
3-Dimethylaminopropylamine	N,N-Dimethyl-1,3-propanediamine; DMAPA	109-55-7	102.18	0.92	Liquid	Amines	Gerberick
3-Ethoxy-1-(2',3',4',5'-tetramethylphenyl)propane-1,3-dione	–	170928-69-5	248.32	3.00	–	–	Gerberick

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
3-Fluoro-5-(3-pyridinyl)benzen-amine	–	181633-36-3	188.21	1.80	Solid	Pharmaceutical chemicals	GSK
3-Hydroxy-2-phenyl-4-quinolinecarboxylic acid	Oxycinchophen	485-89-2	265.27	4.95	Solid	Pharmaceutical chemicals	GSK
3-Hydroxy-4-methoxybenzaldehyde	Isovanillin	621-59-0	152.15	1.28	Solid	Pharmaceutical chemicals	GSK
3-Methyl-4-phenyl-1,2,5-thiadiazole-1,1-dioxide	MPT	3775-21-1	208.24	1.14	–	–	Gerberick
3-Methyleugenol	–	186743-26-0	178.23	2.40	–	Ethers; Phenols	Gerberick
3-Methylisoeugenol	–	186743-29-3	178.23	2.40	–	Carboxylic Acids	Gerberick
3-Phenylenediamine	m-Phenylenediamine	108-45-2	108.14	1.17	Solid	Amines	Gerberick
3-Propoxybenzoic acid	–	190965-42-5	180.21	3.08	Solid	Pharmaceutical chemicals	GSK
3-Propylidenphthalide	–	17369-59-4	174.20	2.40	Liquid	–	Gerberick
4-(Bromomethyl)-benzoic acid ethyl ester	–	26496-94-6	243.10	3.42	–	Pharmaceutical chemicals	GSK
4-(N-Ethyl-N-2-methanesulfamido-ethyl)-2-methyl-1,4-phenylenediamine	CD-4 developer	25646-71-3	836.97	-2.12	Solid	Amides; Sulfur Compounds	Gerberick
4'-(Trifluoro-methyl)-[1,1'-biphenyl]-4-carboxaldehyde	–	90035-34-0	250.22	4.31	Solid	Pharmaceutical chemicals	GSK
4,4,4-Trifluoro-1-phenylbutane-1,3-dione	BFA	362-06-7	219.18	2.52	–	–	Gerberick
4,4-Dibromobenzil	–	35578-47-3	368.02	5.34	Solid	–	LLNA/EC3 Validation Study

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log $K_{ow}^{1,2}$	Physical Form	Chemical Class ³	Data Source
4-[4-[[[(3R)-1-Butyl-3-[(r)-cyclohexyl-hydroxymethyl]-2,5-dioxo-1,4,9-triazaspiro[5.5]-undec-9-yl]methyl]phenoxy]benzoic acid	Aplaviroc	461443-59-4	577.73	3.92	Solid	Pharmaceutical chemicals	GSK
4-Allylanisole	Estragole	140-67-0	148.20	2.54	Liquid	Ethers; Phenols	Gerberick
4-Amino-3-nitrophenyl thiocyanate	–	54029-45-7	195.20	2.21	Solid	Pharmaceutical chemicals	GSK
4-Bromo-1-phthalimidopentane	–	59353-62-7	296.17	3.48	Liquid	Pharmaceutical chemicals	GSK
4-Chloro-6-iodoquinazoline	–	98556-31-1	290.49	2.96	Solid	Pharmaceutical chemicals	GSK
4-Fluoro-2-pyrrolidine-carboxamide	–	748165-40-4	132.14	-1.01	Solid	Pharmaceutical chemicals	GSK
4-Hydroxybenzoic acid	–	99-96-7	138.12	1.03	Solid	Phenols; Carboxylic Acids	Gerberick
4-Iodo-1-phthalimido-pentane	–	63460-47-9	343.17	3.87	Solid	Pharmaceutical chemicals	GSK
4-Isopropyl-1-methylenecyclohexane	–	–	–	–	–	–	LLNA/EC3 Validation Study
4'-Methoxyacetophenone	–	100-06-1	150.18	1.91	Solid	Ethers	Gerberick
4-Methylaminophenol sulfate	Metol; Paramethyl-aminophenol sulfate	55-55-0	344.38	-0.13	Solid	Amines; Phenols	Gerberick
4-Nitrobenzyl bromide	1-(Bromomethyl)-4-nitrobenzene	100-11-8	216.03	1.40	Solid	Hydrocarbons, Cyclic; Nitro Compounds	Gerberick
4-Phenylenediamine	p-PDA, p-Phenylenediamine	106-50-3	108.14	1.17	Solid	Amines	Gerberick

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
5,5-Dimethyl-3-methylenedihydro-2(3H)-furanone	–	29043-97-8	126.16	1.42	–	Heterocyclic Compounds; Sulfur Compounds; Lactones	Gerberick
5-[[4-[(2,3-Dimethyl-2h-indazol-6-yl)-methylamino]-2-pyrimidinyl]amino]-2-methylbenzene-sulfonamide	Pazopanib	444731-52-6	437.53	3.65	Solid	Pharmaceutical chemicals	GSK
5-Amino-2-methylbenzene-sulfonamide	–	69733-09-7	186.23	-0.07	Solid	Pharmaceutical chemicals	GSK
5-Amino-O-Cresol	2-Hydroxy-p-toluidine	2835-95-2	123.15	0.79	Solid	–	NTP
5-Chloro-2,6-dimethoxy-4-methyl-8-nitroquinoline	–	189746-21-2	282.69	3.95	Solid	Pharmaceutical chemicals	GSK
5-Chloro-2,6-dimethoxy-4-methylquinoline	–	189746-19-8	237.69	4.13	Solid	Pharmaceutical chemicals	GSK
5'-Chloro-2'-hydroxy-3'-nitro-[1,1'-biphenyl]-3-carboxylic acid	–	376592-58-4	293.67	4.03	Solid	Pharmaceutical chemicals	GSK
5-Chloro-2-methyl-4-isothiazolin-3-one	–	26172-55-4	149.60	0.92	Liquid	Sulfur Compounds; Heterocyclic Compounds	Gerberick
5-Chloro-6-methoxy-4-methyl-8-nitro-2(1h)quinolinone	–	189746-23-4	268.66	1.99	Solid	Pharmaceutical chemicals	GSK
5-Methoxy-2-nitro-4-(trifluoromethyl)benzene acetonitrile	–	178896-77-0	260.17	2.42	Solid	Pharmaceutical chemicals	GSK
5-Methoxy-6-(trifluoromethyl)-2,3-dihydro-1h-indole	–	178896-79-2	217.19	3.25	Solid	Pharmaceutical chemicals	GSK
5-Methyl-2,3-hexanedione	Acetyl isovaleryl	13706-86-0	128.17	1.42	Liquid	–	Gerberick

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
5-Methyl-2-phenyl-2-hexenal	–	21834-92-4	188.27	3.77	Liquid	–	LLNA/EC3 Validation Study
5-Methyleugenol	–	186743-25-9	178.23	2.40	–	Ethers; Phenols	Gerberick
6-(Diethylamino)-1-hexanol	–	06947-12-2	173.30	1.73	Liquid	Pharmaceutical chemicals	GSK
6-(Trifluoro-methyl)-2,3-dihydro-5-methyl-1h-indole, hydrochloride	–	280121-24-6	237.65	3.69	Solid	Pharmaceutical chemicals	GSK
6-[(2-Methyl-3-pyridinyl)oxy]-3-pyridinamine	–	181633-42-1	201.23	1.42	Solid	Pharmaceutical chemicals	GSK
6-Chloro-1-hexanol	–	2009-83-8	136.62	1.59	Liquid	Pharmaceutical chemicals	GSK
6-Diethylaminohexyl bromide hydrobromide	–	64993-14-2	317.11	3.57	Solid	Pharmaceutical chemicals	GSK
6-Iodo-quinazolin-4-ol	–	16064-08-7	272.05	1.49	Solid	Pharmaceutical chemicals	GSK
6-Methoxy-4-methyl-2(1H)-quinolinone	–	5342-23-4	189.22	1.51	Solid	Pharmaceutical chemicals	GSK
6-Methylcoumarin	6-MC	92-48-8	160.17	2.15	Solid	Heterocyclic Compounds	Gerberick
6-Methyleugenol	–	186743-24-8	178.23	2.40	–	Ethers; Phenols	Gerberick
6-Methylisoeugenol	–	13041-12-8	178.23	2.40	–	Carboxylic Acids	Gerberick
7,12-Dimethylbenz[a]anthracene	DMBA; 9,10-Dimethyl-1,2-benzanthracene	57-97-6	256.34	5.39	Solid	Hydrocarbons, Cyclic; Polycyclic Compounds	Gerberick

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
7-[(4z)-3-(Aminomethyl)-4-(methoxyimino)-1-pyrrolidiny]-1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-1,8-naphthyridine-3-carboxylic acid, monomethane-sulfonate	Gemifloxacin mesylate	210353-53-0	485.50	-1.25	Solid	Pharmaceutical chemicals	GSK
7-Bromotetradecane	7-Tetradecyl bromide; 7-Myristyl bromide	74036-97-8	277.29	4.28	–	Hydrocarbons, Halogenated	Gerberick
8-[(4-Phthalimido-1-methylbutyl)amino]-2,6-dimethoxy-4-methyl-5-(3-trifluoromethylphenoxy)quinoline	–	106635-87-4	593.61	8.70	Solid	Pharmaceutical chemicals	GSK
8-Amino-6-methoxy-4-methylquinoline	–	57514-21-3	188.23	2.30	Solid	Pharmaceutical chemicals	GSK
8-Chloro-3-pentyl-3,7-dihydro-1h-purine-2,6-dione	–	862892-90-8	256.69	2.27	Solid	Pharmaceutical chemicals	GSK
8-Hydroxy-5-[(1r)-1-hydroxy-2-[[2-[4-[(6-methoxy[1,1'-biphenyl]-3-yl)amino]phenyl]-ethyl]amino]ethyl]-2(1h)-quinolinone	–	530084-87-8	521.62	3.98	Solid	Pharmaceutical chemicals	GSK
A SC600	–	–	–	–	–	Formulation	Bayer
Abietic acid	Sylvic acid	514-10-3	302.46	4.61	Solid	Hydrocarbons, Cyclic; Polycyclic Compounds	Gerberick
Adipic acid	1,4-Butanedicarboxylic acid	124-04-9	146.14	-0.02	Solid	Pharmaceutical chemicals	GSK
AE F016382 00 TK71 A101	–	–	–	–	–	Formulation	Bayer

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
Alpha-(p-toluenesulfonyl)-4-fluorobenzyliso-nitrile	–	165806-95-1	289.33	2.04	Solid	Pharmaceutical chemicals	GSK
alpha-Amyl cinnamic aldehyde	–	122-40-7	202.30	3.52	Solid	Aldehydes	Gerberick
alpha-Butyl cinnamic aldehyde	–	7492-44-6	188.27	3.28	Liquid	Aldehydes	Gerberick
alpha-Methyl cinnamic aldehyde	–	101-39-3	146.19	2.54	Liquid	Aldehydes	Gerberick
alpha-Methylphenylacetaldehyde	2-Phenyl propionaldehyde	93-53-8	134.18	2.29	Liquid	Aldehydes	Gerberick
alpha-Phellandrene	Menthadiene; Dihydro-p-cymene; p-Mentha-1,5-diene; 2-methyl-5-(1-methylethyl)- 1,3-cyclohexadiene	99-83-2	136.23	4.62	Solid	Hydrocarbons, Cyclic; Hydrocarbons, Other	LLNA/EC3 Validation Study
alpha-Terpinene	1-Isopropyl-4-methyl-1,3-cyclohexadiene; p-Mentha-1,3-diene	99-86-5	136.23	4.75	Solid	Hydrocarbons, Other	LLNA/EC3 Validation Study
Aniline	Benzenamine	62-53-3	93.13	1.56	Liquid	Amines	Gerberick
Anthranilic acid	–	118-92-3	131.14	1.21	Solid	Pharmaceutical chemicals	GSK
Atrazine SC	–	1912-24-9	215.68	2.82	Solid	Heterocyclic Compounds	ECPA, NTP
Azithromycin	–	83905-01-5	748.99	3.24	Solid	Polycyclic Compounds; Carbohydrates, Lactones	NTP
Bakelite EPR 161	–	9012-45-7	–	–	Solid	Macromolecular substances	BGIA
Bakelite EPR 162	–	9012-45-7	–	–	Solid	Macromolecular substances	BGIA

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
Bakelite EPR 164	–	9012-45-7	–	–	Solid	Macromolecular substances	BGIA
Bandrowski's base	1,4-Cyclohexadiene-1,4-diamine; 1,4-Benzenediamine; N,N"-(2,5-diamino-2,5-cyclohexadiene-1,4-diylidene)bis-(9CI)	20048-27-5	318.38	0.74	Solid	Amines	LLNA/EC3 Validation Study
Basil oil	Ocimum basilicum herb oil	8015-73-4	–	–	Liquid	Lipids	Lalko & Api
Benzaldehyde	–	100-52-7	106.12	1.80	Liquid	Aldehydes	Gerberick
Benzalkonium chloride	–	8001-54-5	–	–	–	Onium Compounds	CESIO
Benzene-1,3,4-tricarboxylic anhydride	Trimellitic anhydride	552-30-7	192.13	0.75	Solid	Anhydrides; Carboxylic Acids	Gerberick
Benzo[a]pyrene	–	50-32-8	252.31	5.39	Solid	Hydrocarbons, Cyclic; Polycyclic Compounds	Gerberick
Benzocaine	–	94-09-7	165.19	1.52	Solid	Carboxylic Acids	Gerberick
Benzoquinone	p-Quinone; 1,4-Cyclohexadienedione	106-51-4	108.10	1.17	Solid	Quinones	Gerberick
Benzyl benzoate	–	120-51-4	212.25	3.14	Liquid	Carboxylic Acids	Gerberick
Benzyl bromide	alpha-Bromotoluene	100-39-0	171.03	2.56	Liquid	Hydrocarbons, Cyclic	Gerberick
Benzylidene acetone	4-phenyl-3-buten-2-one	122-57-6	146.19	2.54	Solid	Ketones	Gerberick
beta-Phellandrene	3-methylene-6-(1-methylethyl)cyclohexene; p-Mentha-1(7),2-diene	555-10-2	136.23	4.70	–	Hydrocarbons, Cyclic; Hydrocarbons, Other	LLNA/EC3 Validation Study

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
beta-Phenylcinnamaldehyde	–	1210-39-5	208.23	2.78	Liquid	–	LLNA/EC3 Validation Study
beta-Propiolactone	–	57-57-8	72.06	0.43	Liquid	Lactones	Gerberick
beta-Terpinene	p-Mentha-1(7),3-diene; (1-methylethyl)-4-methylene-1-cyclohexene	99-84-3	136.23	4.83	–	Hydrocarbons, Other	LLNA/EC3 Validation Study
bis-1,3-(2',5'-dimethylphenyl)-propane-1,3-dione	–	–	282.38	4.37	–	–	Gerberick
Bis-3,4-epoxycyclohexyl-ethyl-phenyl-methylsilane	Ph-Sil	–	–	–	–	–	LLNA/EC3 Validation Study
Bisphenol A-diglycidyl ether	–	1675-54-3	340.42	4.09	Liquid	Ethers	Gerberick
Butyl acrylate	n-butyl acrylate; n-Butyl propenoate; 2-Propenoic acid; Butyl ester	141-32-2	128.17	2.20	Liquid	Carboxylic Acids	NTP, LLNA/EC3 Validation Study
Butyl glycidyl ether	–	2426-08-6	130.19	1.42	Liquid	Ethers	Gerberick
C11-azlactone	–	176665-06-8	267.41	3.24	–	–	Gerberick
C15-azlactone	–	176665-09-1	323.52	4.23	–	–	Gerberick
C17-azlactone	–	176665-11-5	351.58	4.72	–	–	Gerberick
C19-azlactone	–	–	379.63	5.21	–	–	Gerberick
C4-azlactone	–	176664-99-6	169.22	1.52	–	–	Gerberick
C6-azlactone	–	176665-02-4	197.28	2.01	–	–	Gerberick
C9-azlactone	–	176665-04-6	239.36	2.75	–	–	Gerberick
Camphorquinone	Camphoroquinone	465-29-2	166.22	2.15	Solid	Hydrocarbons, Other	Gerberick

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
Chlorobenzene	–	108-90-7	112.56	2.19	Liquid	Hydrocarbons, Cyclic; Hydrocarbons, Halogenated	Gerberick
Chlorothalonil	Tetrachloroisophthalodinitrile	1897-45-6	265.91	3.66	Solid	Nitriles	LLNA/EC3 Validation Study
Cinnamic alcohol	–	104-54-1	134.18	2.29	Solid	Alcohols	Gerberick
Cinnamic aldehyde	Cinnamaldehyde	104-55-2	132.16	2.29	Liquid	Aldehydes	Gerberick
cis-4-Cyano-4-[3-(cyclopentyloxy)-4-methoxyphenyl]cyclohexanecarboxylic acid	Cilomilast	153259-65-5	343.23	3.20	Solid	Pharmaceutical chemicals	GSK
cis-6-Nonenal	–	2277-19-2	140.23	2.29	Liquid	Aldehydes	Gerberick
Citral	3,7-Dimethyl-2,6-octadienal; Geranial-Neral mixture	5392-40-5	152.23	2.54/ 3.45	Liquid	Hydrocarbons, Other	Lalko & Api, Gerberick
Citronella oil	–	8000-29-1	–	–	Liquid	Lipids	Lalko & Api
Clarithromycin	–	81103-11-9	747.95	3.18	Solid	Polycyclic Compounds; Carbohydrates; Lactones	NTP
Clotrimazole	–	23593-75-1	344.84	5.35	Solid	Heterocyclic Compounds	Gerberick
Clove bud oil	Clove oil; Oil of cloves	8000-34-8	–	–	Liquid	Lipids	Lalko & Api
Clove leaf oil	–	8015-97-2	–	–	Liquid	Lipids	Lalko & Api
Clove stem oil	–	8015-98-3	–	–	Liquid	Lipids	Lalko & Api
Coumarin	–	91-64-5	146.15	1.91	Solid	Heterocyclic Compounds	Gerberick
Cyclamen aldehyde	–	103-95-7	190.29	3.28	Liquid	Carboxylic Acids	Gerberick

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
Cytosine	4-Amino-2(1H)-pyrimidinone	71-30-7	120.11	-1.85	Solid	Pharmaceutical chemicals	GSK
D EC25\	–	–	–	–	–	Formulation	Bayer
D EW 15	–	–	–	–	–	Formulation	Bayer
Dicyclohexylcarbodiimide	–	538-75-0	206.33	6.83	Solid	Imines	NTP
Diethyl maleate	–	141-05-9	172.18	0.89	Liquid	Carboxylic Acids	Gerberick
Diethyl sulfate	–	64-67-5	154.19	-0.09	Liquid	Sulfur Compounds	Gerberick
Diethylacetaldehyde	–	97-96-1	100.16	1.56	Liquid	Aldehydes	Gerberick
Diethylenetriamine	–	111-40-0	103.17	0.29	Liquid	Amines	Gerberick
Diethylphthalate	–	84-66-2	222.24	1.87	Liquid	Carboxylic Acids	Gerberick
Dihydroeugenol	2-Methoxy-4-propylphenol; 4-Propylguaicol	2785-87-7	166.22	2.15	Liquid	Ethers; Phenols	Gerberick
Dimethyl 4-cyano-4-(3-cyclopentyloxy-4-methoxyphenyl)-pimelate	–	152630-48-3	403.48	3.31	Solid	Pharmaceutical chemicals	GSK
Dimethyl carbonate	–	616-38-6	90.08	0.10	Liquid	Pharmaceutical chemicals	GSK
Dimethyl sulfate	–	77-78-1	126.13	-0.59	Liquid	Sulfur Compounds	Gerberick
Dimethylsulfoxide	–	67-68-5	78.13	0.57	Liquid	Sulfur Compounds	Gerberick
Dinocap EC	–	39300-45-3	364.39	5.76	Liquid	Hydrocarbons, Cyclic	ECPA
Dipropylene triamine	Bis(3-aminopropyl)amine	56-18-8	131.22	-1.15	Liquid	Amines	BGIA
Dodecyl methanesulfonate	Lauryl methanesulfonate	51323-71-8	264.43	2.51	–	Esters; Sulfur Compounds	Gerberick

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
Endo-tropine-3-mesylate	–	35130-97-3	219.31	-0.11	Solid	Pharmaceutical chemicals	GSK
Ethyl (3-endo)-8-methyl-8-azabicyclo[3.2.1]-octane-3-acetate	–	56880-11-6	211.31	1.53	Liquid	Pharmaceutical chemicals	GSK
Ethyl (z)-alpha-[[2-(1,1-dimethylethoxy)-1,1-dimethyl-2-oxoethoxy]imino]-2-[(triphenylmethyl)amino]-4-thiazoleacetate	–	68672-65-1	599.76	7.75	Solid	Pharmaceutical chemicals	GSK
Ethyl 1h-1,2,4-triazole-3-carboxylate	–	64922-04-9	141.13	-0.02	Solid	Pharmaceutical chemicals	GSK
Ethyl 2,6-dichloro-5-fluoro-beta-oxo-3-pyridinepropanoate	–	96568-04-6	280.09	2.15	Solid	Pharmaceutical chemicals	GSK
Ethyl 4-iodobenzoate	–	51934-41-9	276.08	3.76	Liquid	Pharmaceutical chemicals	GSK
Ethyl benzoylacetate	–	94-02-0	192.21	2.01	Liquid	Esters; Ethers	Gerberick
Ethyl vanillin	–	121-32-4	166.18	1.52	Solid	Aldehydes	Gerberick
Ethyl-2-(Hydroxymethyl)-1,3-Propanediol Triacrylate	–	–	–	–	–	–	NTP
Ethylacrylate	–	140-88-5	100.12	0.92/ 1.22	Liquid	Carboxylic Acids	NTP, Gerberick
Ethylene glycol dimethacrylate	EGDMA	97-90-5	198.22	1.38	Liquid	Carboxylic Acids	Gerberick
Ethylenediamine free base	–	107-15-3	60.10	0.19	Liquid	Amines	Gerberick
Ethylhexyl acrylate	Octyl acrylate; 2-Ethylhexyl 2-propenoate; Acrylic acid; 2-ethylhexyl ester	103-11-7	184.28	4.09	Liquid	Carboxylic Acids	LLNA/EC3 Validation Study

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
Eugenol	2-Methoxy-4-(2-propenyl)phenol; 4-Allyl-2-methoxyphenol; 4-Allylguaiacol	97-53-0	164.20	2.15/ 2.73	Liquid	Carboxylic Acids	Lalko & Api, Gerberick
EXP 10810 A	–	–	–	–	–	Formulation	Bayer
EXP 11120 A	–	–	–	–	–	Formulation	Bayer
F & Fo WG 50 + 25	–	–	–	–	–	Formulation	Bayer
FAR01042-00	–	–	–	–	–	Formulation	Bayer
FAR01060-00	–	–	–	–	–	Formulation	Bayer
Farnesal	–	502-67-0	220.36	3.77	Liquid	Alcohols; Hydrocarbons, other; Lipids	Gerberick
Fatty acid glutamate	–	–	–	–	–	–	CESIO
Fluorescein isothiocyanate	FITC	27072-45-3	389.38	3.32	Solid	Polycyclic Compounds; Isocyanates; Sulfur Compounds	Gerberick
Formaldehyde	–	50-00-0	30.03	0.33/ 0.35	Liquid	Aldehydes	Ryan, Gerberick
Fumaric acid	2-Butenedioic acid; Butenedioic acid; Fumarate	110-17-8	116.07	0.05	Solid	Carboxylic Acids	EFfCI
Furil	–	492-94-4	190.15	1.38	Solid	Heterocyclic Compounds	Gerberick
Fx + Me EW 69	–	–	–	–	–	Formulation	Bayer
Geraniol	Rhodinol	106-24-1	154.25	2.54/ 3.47	Liquid	Hydrocarbons, Other	Lalko & Api, Gerberick
Geranium oil	Pelargonium oil	8000-46-2	–	–	Liquid	–	Lalko & Api
Glutaraldehyde	–	111-30-8	100.12	0.92	Liquid	Aldehydes	Gerberick

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log $K_{ow}^{1,2}$	Physical Form	Chemical Class ³	Data Source
Glycerol	–	56-81-5	92.09	0.05	Liquid	Alcohols; Carbohydrates	Gerberick
Glyceryl thioglycolate	Acetic acid, mercapto-, monoester with 1,2,3-propanetriol	30618-84-9	166.19	-1.29	–	Lipids	CESIO
Glyoxal	Oxaldehyde; Ethanedial; Biformyl	107-22-2	58.04	0.19	Liquid	Aldehydes	Gerberick
Hexane	–	110-54-3	86.18	1.94	Liquid	Hydrocarbons, Acyclic	Gerberick
Hexyl cinnamic aldehyde	HCA; alpha-Hexyl-cinnamaldehyde; 2-(Phenylmethylene) octanal	101-86-0	216.32	3.77/ 4.82	Liquid	Aldehydes	BGIA, Gerberick
Hydroxycitronellal	–	107-75-5	172.26	2.15	Liquid	Hydrocarbons, Other	Gerberick
Hydroxyethylethylenediamine	N-(2-Hydroxyethyl) ethylenediamine	111-41-1	104.15	-2.13	Liquid	Alcohols; Amines	BGIA
Imidazolidinyl urea	Germall 115, Imidurea	39236-46-9	388.29	-3.00	Solid	Urea	Gerberick
Iodopropynyl butylcarbamate	3-iodo-2-propynylbutyl-carbamate	87977-28-4	281.09	2.45	Solid	Carboxylic Acids	LLNA/EC3 Validation Study
Isoeugenol	2-Methoxy-4-propenylphenol; 4-Propenylguaiaicol	97-54-1	164.20	2.15	Liquid	Carboxylic Acids	Gerberick
Isononanoyl chloride	–	57077-36-8	176.69	2.54	–	Carboxylic Acids	Gerberick
Isopropanol	Isopropyl alcohol, 2-Propanol	67-63-0	60.10	0.82	Liquid	Alcohols	Gerberick
Isopropyl dicyandiamide	–	35695-36-4	126.16	0.51	Solid	Pharmaceutical chemicals	GSK
Isopropyl myristate	–	110-27-0	270.46	3.88	Liquid	Lipids	Gerberick
Isopropyleugenol	–	51474-90-9	206.29	2.89	–	Ethers; Phenols	Gerberick
Isopropylisoeugenol	–	2953-00-7	206.29	2.89	–	Ethers	Gerberick

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
Jasmine absolute (Grandiflorum)	Jasmine oil	8022-96-6	–	–	Liquid	Lipids	Lalko & Api
Jasmine absolute (Sambac)	Jasmine oil	8022-96-6	–	–	Liquid	Lipids	Lalko & Api
Kanamycin	–	59-01-8; 8063-07-8	484.50	-0.90	Solid	Carbohydrates	Gerberick
Lactic acid	2-Hydroxypropanoic acid	598-82-3	90.08	0.05	Liquid	Carboxylic Acids	Gerberick
Lauryl gallate	–	1166-52-5	338.44	3.21	Solid	Carboxylic Acids	Gerberick
Laurylglycerin derivitive	–	–	–	–	–	–	CESIO
Lemongrass oil	Citral terpenes; Indian melissa oil; Indian oil of verbena; Cymbopogon citratus oil	8007-02-1	–	–	Liquid	Lipids; Hydrocarbons, other	Lalko & Api
Linalool alcohol	Linalool; Linalol; Linalyl alcohol	78-70-6	154.25	2.54/ 3.38	Liquid	Hydrocarbons	Gerberick, LLNA/EC3 Validation Study
Linalool aldehyde	–	–	–	–	–	–	LLNA/EC3 Validation Study
Linoleic acid	Grape seed oil	60-33-3	280.45	7.51	Liquid	Lipids	EFfCI
Linolenic acid	9,12,15-Octadecatrienoic acid	463-40-1	278.43	7.30	Liquid	Lipids	EFfCI
Litsea cubeba oil	–	68855-99-2	–	–	Liquid	–	Lalko & Api
Maleic acid	cis-Butenedioic acid; Toxicic acid	110-16-7	116.07	0.05	Solid	Carboxylic Acids	EFfCI
m-Chloropropio-phenone	3'-Chloropropiophenone	34841-35-5	168.62	2.90	Solid	Pharmaceutical chemicals	GSK
Methyl 4-(bromomethyl)benzoate	–	2417-72-3	229.08	2.89	Solid	Pharmaceutical chemicals	GSK

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
Methyl 4-(bromomethyl)benzoate	–	2417-72-3	229.08	2.89	Solid	Pharmaceutical chemicals	GSK
Methyl acrylate	Methyl propenoate; Acrylic acid methyl ester; Methoxy-carbonylethylene	96-33-3	86.09	0.73	Liquid	Carboxylic Acids	LLNA/EC3 Validation Study
Methyl dodecanesulfonate	–	2374-65-4	264.43	2.51	–	Esters; Sulfur Compounds	Gerberick
Methyl hexadecyl sulfonate	–	4230-15-3	320.53	3.49	–	Hydrocarbons, Acyclic; Sulfur Compounds	Gerberick
Methyl hexadecenesulfonate	–	26452-48-2	318.52	3.49	–	Ethers; Sulfur Compounds	Gerberick
Methyl methanesulfonate	–	66-27-3	110.13	-0.20	Liquid	Hydrocarbons, Acyclic; Sulfur Compounds	Gerberick
Methyl pyruvate	–	600-22-6	102.09	-0.96	Liquid	Carboxylic Acids	LLNA/EC3 Validation Study
Methyl salicylate	Oil of wintergreen, 2-Hydroxybenzoic acid methyl ester	119-36-8	152.15	1.28/2.60	Liquid	Phenols; Carboxylic Acids	NTP, Gerberick
Methyl(2-sulfomethyl) octadecanoate	–	–	454.67	4.89	–	Ethers; Sulfur Compounds	Gerberick
Methyl-2-nonynoate	–	111-80-8	168.24	2.15	Liquid	Lipids	Gerberick
Methyl-4-hydroxybenzoate	Methylparaben	99-76-3	152.15	1.28	Solid	Carboxylic Acids	Gerberick
Methylmethacrylate	Pegalan	80-62-6	100.12	1.28	Liquid	Carboxylic Acids; Macromolecular Substances	LLNA/EC3 Validation Study

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
m-Phenylenebis(methylamine)	1,3-xylenediamine; m-Xylylenediamine; 1,3-Bis(aminomethyl)-benzene	1477-55-0	136.19	0.15	Liquid	Hydrocarbons, Cyclic	BGIA
n-(2-Chloro-4-pyrimidinyl)-2,3-drimethyl-2h-indazol-6-amine	–	444731-74-2	273.73	3.02	Solid	Pharmaceutical chemicals	GSK
n-(2-Chloro-4-pyrimidinyl)-n,2,3-trimethyl-2h-indazol-6-amine	–	444731-75-3	287.75	2.88	Solid	Pharmaceutical chemicals	GSK
n-(3,4-Dichlorophenyl)-n'-(1-methylethyl)-imidodicarbonimidic diamide monohydrochloride	Chlorproguanil hydrochloride	15537-76-5	324.64	3.22	Solid	Pharmaceutical chemicals	GSK
n-(4-Methoxyphenyl)-3-oxobutanamide	–	5437-98-9	207.23	0.88	Solid	Pharmaceutical chemicals	GSK
n-[(1,1-Dimethylethoxy)-carbonyl]-l-tyrosine, ethyl ester	–	72594-77-5	309.37	2.66	Solid	Pharmaceutical chemicals	GSK
n-[(1-Butyl-4-piperidinyl)methyl]-3,4-dihydro-2h-[1,3]oxazino[3,2-a]indole-10-carboxamide	Piboserod	152811-62-6	369.51	4.01	Solid	Pharmaceutical chemicals	GSK
n-[2-(Diethylamino)ethyl]-2-[[[(4-fluorophenyl)-methyl]thio]-4,5,6,7-tetrahydro-4-oxo-n-[[4'-(trifluoromethyl)-[1,1'-biphenyl]-4-yl]methyl]-1h-cyclopentapyrimidine-1-acetamide	–	356057-34-6	666.79	8.33	Solid	Pharmaceutical chemicals	GSK
n-[2-Benzyloxy-5-(2-bromo-1-hydroxy-ethyl)-phenyl]-formamide	–	201677-59-0	350.22	2.51	Solid	Pharmaceutical chemicals	GSK

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
n-{{[(1,1-Dimethylethyl)oxy]carbonyl}-4-fluoro-beta-(4-fluorophenyl)-l-phenylalanine	–	481055-29-2	377.39	4.31	Solid	Pharmaceutical chemicals	GSK
n-Amino-pyridinium	–	35073-04-2	223.02	0.35	Solid	Pharmaceutical chemicals	GSK
N-Ethyl-N-nitrosourea	ENU	759-73-9	117.11	-0.73	Solid	Nitroso Compounds; Urea	Gerberick
Nickel Sulfate	–	7786-81-4	154.76	-0.17	–	Inorganic Chemical, Metals; Inorganic Chemical, Elements	Ryan
n-Isopropyl-n-phenyl-2-(2-phenylamino-phenylamino)-acetamide	–	161455-90-9	359.48	4.91	Solid	Pharmaceutical chemicals	GSK
N-Methyl-N-nitrosourea	MNU	684-93-5	103.08	-0.97	Solid	Nitroso Compounds; Urea	Gerberick
Nonanoyl chloride	Pelargonoyl chloride	764-85-2	176.68	2.54	Liquid	Carboxylic Acids	Gerberick
Non-ionic surfactant 1	–	–	–	–	–	–	CESIO
Non-ionic surfactant 2	–	–	–	–	–	–	CESIO
Non-ionic surfactant 3	–	–	–	–	–	–	CESIO
Non-ionic surfactant 4	–	–	–	–	–	–	CESIO
Non-ionic surfactant 5	–	–	–	–	–	–	CESIO
Non-ionic surfactant 6	–	–	–	–	–	–	CESIO
Non-ionic surfactant 7	–	–	–	–	–	–	CESIO
Non-ionic surfactant 8	–	–	–	–	–	–	CESIO
Non-ionic surfactant 9	–	–	–	–	–	–	CESIO

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
Norbornene fluoroalcohol	2[(bicyclo[2.2.1]hept-5-ene-2-yloxy)methyl]-1,1,1,3,3,3-hexafluoro-2-propanol	305815-63-8	290.20		Liquid	–	LLNA/EC3 Validation Study
Octanoic acid	–	124-07-2	144.21	1.66	Liquid	Carboxylic Acids; Lipids	Gerberick
Octinol	Capryl alcohol; Octyl alcohol	111-87-5	130.23	2.81	Liquid	Alcohols; Lipids	EFfCI
Oleic acid	cis-9-Octadecenoic acid; Elainic acid	112-80-1	282.46	7.73	Liquid	Lipids	EFfCI
Oleyl methane sulfonate	–	35709-09-2	346.57	3.98	Liquid	Hydrocarbons, Acyclic; Sulfur Compounds	Gerberick
Oripavine	Oripavine	467-04-9	297.36	1.21	Solid	Pharmaceutical chemicals	GSK
Oxalic acid	–	144-62-7	90.03	-0.59	Solid	Carboxylic Acids	Gerberick
Oxazolone	4-Ethoxymethylene-2-phenyloxazol-5-one	15646-46-5	217.22	1.87	Solid	Heterocyclic Compounds	Gerberick
Oxirane, mono((C12-14-alkyloxy)methyl) derivs	–	68609-97-2	–	–	Liquid	–	BGIA
Oxyfluorfen EC	–	42874-03-3	361.70	5.21	Solid	Ethers	ECPA
Palmarosa oil	Cymbopogon martini oil; Geranium oil, east indian	8014-19-5	–	–	Liquid	–	Lalko & Api
Palmitoyl chloride	–	112-67-4	274.88	4.26	Liquid	Lipids	Gerberick
Penicillin G	–	61-33-6	334.39	2.09	Solid	Amides; Sulfur Compounds; Heterocyclic Compounds	Gerberick
Pentachlorophenol	Penta; PCP	87-86-5	266.34	2.79	Solid	Phenols	Gerberick

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
Pentaerythritol Triacrylate	–	3524-68-3	298.29	0.91	–	Carboxylic Acids, Alcohols	NTP
Perillaldehyde	–	2111-75-3	150.22	2.54	Liquid	Hydrocarbons, Other	Gerberick
Phenyl benzoate	–	93-99-2	198.22	2.89	Solid	Carboxylic Acids	Gerberick
Phenylacetaldehyde	–	127-78-1	120.15	2.05	Liquid	Aldehydes	Gerberick
Phenylmethyl 2-(4-fluoro-2-methylphenyl)-4-oxo-3,4-dihydro-1(2h)-pyridine-carboxylate	–	414909-98-1	339.37	3.94	Solid	Pharmaceutical chemicals	GSK
Pluronic L92\	–	–	–	–	–	–	Ryan
p-Methylhydrocinnamic aldehyde	p-Cresyl propionaldehyde	5406-12-2	148.21	2.54	Liquid	–	Gerberick
Potassium dichromate	PDC	7778-50-9	294.18	0.62	Solid	Inorganic Chemical, Chromium Compounds; Inorganic Chemical, Potassium Compounds	NTP, Ryan, Gerberick
Precursor surfactant 1	–	–	–	–	–	–	CESIO
Precursor surfactant 2	–	–	–	–	–	–	CESIO
Propylene glycol	1,2-Dihydroxypropane; 1,2-Propanediol	57-55-6	76.09	0.43	Liquid	Alcohols	Gerberick
Propylparaben	Propyl 4-hydroxybenzoate	94-13-3	180.20	1.77	Solid	Phenols; Carboxylic Acids	Gerberick
p-tert-Butyl-a-ethyl-hydrocinnamal	Lilial	80-54-6	204.31	3.52	Liquid	Aldehydes	Gerberick
p-tert-Butylphenylglycidylether	4-tert-Butylphenyl 2,3-epoxypropyl ether	3101-60-8	206.28	3.52	Liquid	–	BGIA

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
Pyridine	–	110-86-1	79.10	1.31	Liquid	Heterocyclic Compounds	Gerberick
Quinoxifen SC	–	124495-18-7	308.13	5.69	Liquid	Heterocyclic Compounds	ECPA
Quinoxifen/cyproconazole	–	124495-18-7/ 113096-99-4	308.134/291.776	5.69/3.25	Liquid	Heterocyclic Compounds	ECPA
R(+)-Limonene	–	5989-27-5	136.24	2.93	Liquid	Hydrocarbons; Hydrocarbons, Cyclic	Gerberick
R-Carvone	–	2244-16-8	150.22	3.07	Liquid	Hydrocarbons, Other	LLNA/EC3 Validation Study
R-Carvoxime	–	2051-55-0	165.23	3.57	Solid	–	LLNA/EC3 Validation Study
rel-(3r,3as,6ar)-Hexahydrofuro[2,3-b]furan-3-yl 4-nitrophenyl carbonate	–	252873-35-1	295.25	0.83	Solid	Pharmaceutical chemicals	GSK
Resorcinol	1,3-Dihydroxybenzene	108-46-3	110.11	1.17	Solid	Phenols	Basketter
Rifamycin SV	–	14897-39-3	697.77	5.04	Solid	Heterocyclic Compounds, Polycyclic Compounds	NTP
Saccharin	–	81-07-2	183.18	0.64	Solid	Sulfur Compounds; Heterocyclic Compounds	Gerberick
Salicylic acid	2-Hydroxybenzoic acid	69-72-7	138.12	1.03	Solid	Phenols; Carboxylic Acids	Gerberick
Saturated diglycerin	–	–	–	–	–	–	CESIO
Sodium ethyl xanthate	Carbonodithioic acid, O-ethyl ester, sodium salt	140-90-9	144.19	2.11	Solid	Pharmaceutical chemicals	GSK

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
Sodium lauroyl lactylate	Pationic 138C	13557-75-0	366.43	2.58	–	–	Gerberick
Sodium lauryl sulfate	Sodium dodecyl sulfate, SLS, SDS, Irium	151-21-3	288.38	1.87/ 1.69	Solid	Alcohols; Sulfur Compounds; Lipids	BGIA, Gerberick
Sodium metasilicate	–	6834-92-0	122.06	-5.65	–	Minerals, Silicon Compounds	NTP
Sodium-3,3,5-trimethylhexanoyloxy-benzenesulfonate	–	94612-91-6	336.38	2.23	–	–	Gerberick
Spearmint oil	–	68917-46-4	–	–	Liquid	–	Lalko & Api
Squalene	2,6,10,15,19,23-Hexamethyl-2,6,10,14,18,22-tetracosahexaene	111-02-4	410.72	14.12	Liquid	Hydrocarbons, Acyclic	EFfCI
Streptomycin sulfate	–	3810-74-0	1457.39	-8.50	Solid	Carbohydrates	Gerberick
Succinic acid	Butanedioic acid	110-15-6	118.09	-0.75	Solid	Carboxylic Acids	EFfCI
Sulfanilamide	4-Aminobenzene-sulfonamide; p-Anilinesulfonamide; p-Sulfamidoaniline	63-74-1	172.21	0.40	Solid	Amides; Sulfur Compounds; Amines	Gerberick
Sulfanilic acid	p-Aminobenzene-sulfonic acid; p-Anilinesulfonic acid	121-57-3	173.19	0.40	Solid	Hydrocarbons, Cyclic; Sulfur Compounds	Gerberick
Tartaric acid	[R-(R*,R*)]-2,3-Dihydroxybutanedioic acid; L-Tartaric acid	87-69-4	150.09	0.87	Solid	Alcohols; Carboxylic Acids	Gerberick
tert-Butyl-3-aminobenzoate	–	92146-82-2	193.25	2.63	Solid	Pharmaceutical chemicals	GSK
Tetramethyl thiuram disulfide	Thiram; Bis (dimethylthio-carbamoyl) disulfide	137-26-8	240.44	1.17	Solid	Carboxylic Acids; Sulfur Compounds	Gerberick

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
trans-2-Decenal	–	3913-71-1	154.25	2.54	Liquid	Aldehydes; Hydrocarbons, Other	Gerberick
trans-2-Hexenal	–	6728-26-3	98.15	1.56	Liquid	Heterocyclic Compounds	Gerberick
Trans-2-methyl-2-butenal	–	497-03-0	84.12	1.15	Liquid	Aldehydes	LLNA/EC3 Validation Study
trans-Anethol	–	104-46-1	148.21	2.54	Liquid	Ethers; Phenols	Gerberick
Trienol	17,21-Dihydroxy-16beta-methylpregna-1,4,9(11)-triene-3,20-dione	13504-15-9	356.47	3.02	Solid	Pharmaceutical chemicals	GSK
Trifluralin EC	–	1582-09-8	335.28	5.31	–	Hydrocarbons, Cyclic; Amine	ECPA
Trimethylhexamine diamine	–	–	–	–	–	–	BGIA
Trimethylolpropane Triacrylate	–	15625-89-5	296.32	2.86	Liquid	Carboxylic Acids	NTP
Undec-10-enal	–	112-45-8	168.28	2.79	Liquid	Aldehydes	Gerberick
Undecylenic acid	10-Undecenoic acid	112-38-9	184.28	4.37	Liquid	Lipids	EFfCI
Unsaturated fatty acid	–	–	–	–	–	–	CESIO
Unsaturated fatty acid ester	–	–	–	–	–	–	CESIO
Vanillin	–	121-33-5	152.15	1.28	Solid	Aldehydes	Gerberick
Veratraldehyde	–	120-14-9	166.18	1.45	Solid	Pharmaceutical chemicals	GSK
Vinylidene dichloride	–	75-35-4	96.94	1.45	Liquid	Hydrocarbons, Acyclic; Hydrocarbons, Halogenated	Gerberick
Vinylpyridine	Ethylene-pyridine	1337-81-1	105.14	1.80	Liquid	Heterocyclic Compounds	Gerberick

Substance Name	Synonyms	CASRN	Mol. Weight (g/mol)	Log K _{ow} ^{1,2}	Physical Form	Chemical Class ³	Data Source
Ylang Ylang (Extra)	Cananga oil; Canangium odoratum genuina oil	8006-81-3	–	–	Liquid	–	Lalko & Api
Ylang Ylang (III)	Cananga oil; Canangium odoratum genuina oil	8006-81-3	–	–	Liquid	–	Lalko & Api

Abbreviations: CASRN = Chemical Abstracts Service Registry Number; g/mol = grams per mole.

¹ K_{ow} represents the octanol-water partition coefficient (expressed on log scale).

² When two numbers are shown for K_{ow}, the first number is the value calculated by the method of Moriguchi et al. (1994) and provided in Gerberick et al. (2005). The second number was calculated by the method of Meylan and Howard (1995) and obtained from the website: <http://www.srcinc.com/what-we-do/databaseforms.aspx?id=385>. LogP (log K_{ow}) values for GSK chemicals were calculated using the method provided by Daylight Chemical Information Systems (see: <http://www.daylight.com/dayhtml/doc/clogp/index.html>).

³ Chemical classifications based on the Medical Subject Headings classification for chemicals and drugs, as developed by the National Library of Medicine (available at <http://www.nlm.nih.gov/mesh/meshhome.html>). Chemical classification of "pharmaceutical chemicals" for the GSK chemicals was suggested by Dr. Michael Olson of GSK, which in spirit captures three types of pharmaceutical active substances (actives, intermediates, and starting materials).

⁴ Basketter = Basketter et al. 2007; Bayer = Bayer CropScience SA Studies, submitted by E. Debruyne; BGIA = Berufsgenossenschaftliches Institut für Arbeitsschutz (German Institute for Occupational Safety and Health) Study Report, submitted by H.W. Vohr; CESIO = Comité Européen des Agents de Surface et de Leurs Intermediaires Organiques (European Committee of Surfactants and Their Organic Intermediates) Report, submitted by K. Skirda; ECPA = European Crop Protection Association LLNA Project Report, submitted by P. Botham; EFfCI = European Federation for Cosmetic Ingredients study, submitted by P. Ungeheuer; Gerberick = Gerberick et al. 2005; GSK = Glaxo SmithKline, submitted by M.J. Olson; Lalko & Api = Lalko & Api (2006), submitted by A. Api (Research Institute for Fragrance Materials [RIFM]); LLNA/EC3 Validation Study, submitted by D. Basketter, I. Kimber, and F. Gerberick; NTP = NTP Study, submitted by D. Germolec; Ryan = Ryan et al. (2002).