

No.	Chemical	Class	CAS No.	Supplier	Physical state	Density (g/cm ³)	logP	pH ^a	GHS ^b	EPA ^c	Draize score				Temperature (°C)	Scores ^d			Result of Phase III variation study					
											Score	Ref.	Test date	Protocol ver.		Lag time	Intensity	Plateau level	Judgment ^e	chemical No.	FDSC	BoZo	Daicel	
1	Cyclohexanol	Alcohols	108-93-0	Sigma-Aldrich	Liquid	0.96	1.23	7	1	I	79.8	g	2011/9/15	*	30	0	0.31	56.0	I					
2	Sodium salicylate	Organic salts	54-21-7	Wako	Solid	0.32	0.42	7	1	I	83.7	h	2011/10/20	*	30	0	1.01	60.0	I	3-32	I	I	I	
3	Triton X-100	Surfactants (nonionic)	9002-93-1	Sigma-Aldrich	Liquid	1.06	4.89	7	1	I	68.7 ^g	g	2011/10/16	*	30	0	0.92	83.0	I					
4	Diethylethanolamine	Amines	100-37-8	Sigma-Aldrich	Liquid	0.88	0.21	10	1	I	94.7	i	2018/3/20	1.8e	27	10	0.62	107.0	I					
5	m-Phenylendiamine	Amines	108-45-2	Wako	Solid	1.14	-0.33	8	1	I	-	-	2018/3/20	1.8e	27	10	0.46	78.0	I	3-9	I	I	I	
6	Imidazole	Heterocyclics	288-32-4	Sigma-Aldrich	Solid	1.03	-0.08	9	1	I	59.3	g	2014/9/30	1.8e	28	110	0.22	17.0	I	3-30	I	I	I	
7	Disteardimethylammonium chloride	Surfactants (cationic)	107-64-2	Wako	Solid	0.86	1.01	7	1	I	96.3	h	2013/7/9	1.3e	28	90	0.03	1.0	I					
8	Promethazine hydrochloride	Miscellaneous	58-33-3	Sigma-Aldrich	Solid	-	4.96	6	1	I	71.3	g	2018/4/3	1.8e	28	0	0.77	138.0	I					
9	Benzyl alcohol	Alcohols	100-51-6	Sigma-Aldrich	Liquid	1.05	1.10	7	1	I	31	h	2018/3/20	1.8e	29	0	0.44	79.0	I					
10	Acid red 92	Color additives	18472-87-2	Wako	Solid	2.16	7.13	unmeasurable	1	I	71	h	2012/4/27	*	28	0	0.74	82.0	I					
11	Lactic acid	Carboxylic acids	50-21-5	Alfa Aesar	Liquid	1.20	-0.72	3	1	I	102.7	i	2013/11/19	1.4e	27	>180	-0.30	0.0	NI					
12	Calcium thioglycolate	Organic salts	814-71-1	Wako	Solid	1.31	0.11	10	1	-	52.3	i	2018/4/3	1.8e	28	0	2.32	116.0	I					
13	2-Benzyl-4-chlorophenol	Phenol	120-32-1	Wako	Solid	1.19	2.60	7	1	I	-	-	2015/3/10	1.8e	28	0	0.31	55.8	I	3-2	I	I	I	
14	Capta	Heterocyclic compound, Sulfur compound (organic)	133-06-2	TCI	Solid	1.74	2.80	7	1	I	83	g	2015/3/10	1.8e	28	>180	-0.04	0.0	NI	3-4	NI	NI	NI	
15	3-(2-Aminoethylamino)propyltrimethoxysilane	Silicon compound	1760-24-3	Aldrich	Liquid	1.01	-1.00	10	1	-	-	-	2015/3/3	1.8e	28	30	0.17	27.6	I	3-7	I	I	I	
16	Tetraethylene glycol	Acrylate, Ester	17831-71-9	TCI	Liquid	1.13	1.26	7	1	-	-	-	2015/3/24	1.8e	28	0	0.20	36.7	I	3-10	I	I	I	
17	Triethanolamine polyoxyethylene (3) lauryl ether sulfate, 40%	Surfactants (cationic)	27028-82-6	KAO	Liquid	1.07	-	7	1	-	-	-	2018/5/29	1.8e	26	0	0.51	92.0	I					
18	Sodium polyethylene (3) lauryl ether sulfate, 25.5%	Surfactants (cationic)	9004-82-4	KAO	Liquid	1.05	-	7	1	-	-	-	2018/5/29	1.8e	28	0	0.47	85.0	I					
19	Polyoxyethylene (10) polyoxypropylene (1.5) lauryl-mystyl ether	Surfactants (nonionic)	68439-51-07	KAO	Liquid	1.01	-	6	1	-	-	-	2018/5/29	1.8e	28	0	0.45	82.0	I					
20	Basasol Orange 52L	Color additives	-	BASF	Liquid	-	-	unmeasurable	1	-	-	-	2018/5/29	1.8e	29	0	0.27	49.0	I					
21	Cetylpyridinium bromide (10%)	Surfactants (cationic)	140-72-7	Kanto	Liquid	-	1.77	7	1	-	89.7	g	2018/5/29	1.8e	28	0	0.41	74.0	I					
22	Acetic acid (10%)	Carboxylic acids	64-19-7	Kanto	Liquid	1.05	-0.17	4	1	-	-	-	2018/5/29	1.8e	27	>180	-0.48	0.0	NI					
23	Cetyltrimethylammonium bromide (10%)	Surfactants (cationic)	57-09-0	Kanto	Liquid	-	1.01	7	1	-	-	-	2018/5/29	1.8e	29	0	0.46	83.0	I					
24	Stearyltrimethylammonium chloride (10%)	Surfactants (cationic)	112-03-8	Wako	Liquid	0.89	1.01	7	1	-	-	-	2018/5/29	1.8e	29	0	0.37	66.0	I					
25	Domiphen bromide (10%)	Surfactants (cationic)	538-71-6	Sigma-Aldrich	Liquid	-	2.91	7	1	-	-	-	2018/6/5	1.8e	27	0	0.47	85.0	I					
26	Cetylpyridinium chloride (10%)	Surfactants (cationic)	6004-24-6	Kanto	Liquid	1.00-1.12	1.77	7	1	-	-	-	2018/6/5	1.8e	27	0	0.43	78.0	I					
27	Benzethonium chloride (10%)	Surfactants (cationic)	121-54-0	Kanto	Liquid	1.00	2.90	7	1	-	108	g	2018/6/5	1.8e	28	0	0.49	88.0	I					
28	Butyl cellosolve	Alcohols	111-76-2	Sigma-Aldrich	Liquid	0.90	0.83	8	2	or higher	II	68.7	g	2012/4/27	*	28	0	0.48	58.0	I				
29	Dodecanoic acid	Carboxylic acid	143-07-7	Sigma-Aldrich	Solid	0.88	-	6	2	-	-	-	2018/5/29	1.8e	27	50	0.28	36.0	I					
30	Ethanol	Alcohols	64-17-5	Wako	Liquid	0.79	-0.31	7	2A	or higher	I	24	g	2018/3/9	1.8e	26	0	0.22	39.0	I				
31	Nonylphenyl-polyethylene glycol	Polysols	9016-45-9	Wako	Solid	1.06	6.51	7	2A	or higher	-	-	2014/7/15	1.6e	28	40	0.20	30.1	I					
32	Butanol	Alcohols	71-36-3	Wako	Liquid	0.81	0.88	8	2A	or higher	I	60.8	g	2012/4/27	*	28	0	0.89	53.0	I	3-6	I	I	I
33	Pyridine	Heterocyclic compounds	110-86-1	Sigma-Aldrich	Liquid	0.98	0.65	7	2A	or higher	I	48	g	2018/4/3	1.8e	27	0	0.32	57.0	I				
34	Isobutyl alcohol	Alcohols	78-83-1	Wako	Liquid	0.81	0.76	7	2A	or higher	I	60.3	i	2013/11/19	1.4e	27	10	0.24	44.1	I				
35	2-Ethyl-1-hexanol	Alcohols	104-76-7	Wako	Liquid	0.83	3.04	7	2A	II	51.3	g	2011/9/15	*	30	0	0.23	41.0	I					
36	Isopropyl alcohol	Alcohols	67-63-0	Wako	Liquid	0.78	0.05	7	2A	III	30.5	g	2011/9/15	*	30	0	0.30	27.0	I					
37	n-Hexanol	Alcohols	111-27-3	Sigma-Aldrich	Liquid	0.82	2.03	7	2A	II	64.8	g	2011/9/15	*	30	0	0.33	59.0	I					
38	Acetone	Ketones	67-64-1	Wako	Liquid	0.79	-0.24	7	2A	II	65.8	g	2011/10/20	*	30	0	0.21	10.0	I					
39	Methyl ethyl ketone	Ketones	78-93-3	TCI	Liquid	0.81	0.29	7	2A	III	50	g	2018/3/20	1.8e	27	0	0.31	56.0	I					
40	Propasol solvent P	Alcohols	1569-01-3	Sigma-Aldrich	Liquid	0.89	0.56	8	2A	II	-	-	2012/4/27	*	28	0	0.38	57.0	I	3-20	I	I	I	
41	3,3'-Dithiodipropionic acid	Acids	1119-62-6	Wako	Solid	1.45	-0.15	4	2A	II	31.7	g	2013/10/29	1.4e	28	>180	-0.02	0.0	NI					
42	Ammonium nitrate	Organic salts	6484-52-2	Sigma-Aldrich	Solid	1.72	-	8	2A	III	18.3	g	2012/4/27	*	28	0	2.07	62.0	I					
43	Methyl cyanoacetate	Esters, Nitrile compounds	105-34-0	Sigma-Aldrich	Solid	1.12	-0.47	7	2A	II	27.7	g	2013/10/29	1.4e	28	20	0.07	14.0	I					
44	Cyclopentanol	Alcohols	96-41-3	Sigma-Aldrich	Liquid	0.95	2.41	7	2A	II	21.7	h	2018/4/3	1.8e	26	10	0.33	57.0	I	3-37	I	I	I	
45	Butyrolactone	Heterocyclic compounds, Ketones	96-48-0	Sigma-Aldrich	Liquid	1.13	-0.64	7	2A	II	43	g	2018/3/20	1.8e	28	10	0.26	46.0	I	3-11	I	I	I	
46	2,6-Dichlorobenzoyl chloride	Acyl halide	4659-45-4	Sigma-Aldrich	Liquid	1.47	2.54	3	2A	II	23.8	g	2015/3/10	1.8e	28	110	0.35	24.7	I	3-14	NI	I	NI	
47	Dibenzyl phosphate	Organophosphorus compound	1623-08-1	TCI	Solid	1.46	1.71	3	2A	II	30	g	2015/3/10	1.8e	28	0	0.34	61.0	I	3-15	I	I	I	
48	Potassium oleate	Fatty acid salt	143-18-0	Sigma-Aldrich	Solid	1.10	3.92	9	2A	-	-	-	2018/5/29	1.8e	28	0	0.69	83.0	I					
49	Hydroxyethylcellulose ethoxylate, quaternized	Ester, Ammonium salt	68610-92-4	Sigma-Aldrich	Solid	-	-	7	2A	-	-	-	2018/5/29	1.8e	28	10	0.28	5.0	I					
50	1-Octanol	Alcohols	111-87-5	Wako	Liquid	0.83	3.00	7	2B	or higher	IV	41	g	2018/3/20	1.8e	28	120	0.18	32.0	I				
51	Methyl acetate	Esters	79-20-9	Sigma-Aldrich	Liquid	0.93	0.18	7	2B	or higher	II	39.5	g	2013/11/19	1.4e	27	10	0.16	29.2	I	3-12	I	I	I
52	2-Methyl-1-pentanol	Alcohols	105-30-6	TCI	Liquid	0.83	1.76	7	2B	III	13	g	2011/9/15	*	30	0	0.77	46.0	I	3-31	I	I	I	
53	n-Butanol	Aldehydes	123-72-8	Sigma-Aldrich	Liquid	0.80	0.88	7	2B	III	-	-	2018/4/3	1.8e	26	10	0.32	56.0	I					
54	Camphene	Hydrocarbons	79-92-5	Sigma-Aldrich	Solid	0.84	1.94	7	2B	III	-	-	2013/10/29	1.4e	28	100	0.04	4.0	I	3-18	I	NI	NI	
55	Ethyl 2,6-dichloro-5-fluoro-beta-oxo-3-pyridinepropanoate	Esters	96568-04-6	TCI	Solid	1.43	2.30	5	2B	III	-	-	2013/10/29	1.4e	28	>180	0.00	1.0	NI					
56	3-Chloropropionitrile	Nitriles	542-76-7	Wako	Liquid	1.16	0.18	5	2B	III	13.7	g	2013/7/9	1.3e	28	10	0.31	56.0	I					
57	Di(propylene glycol) propyl ether	Alkoxylated alcohol	2991-17-1	Sigma-Aldrich	Liquid	0.94	1.14	7	2B	III	-	-	2018/3/20	1.8e	28	10	0.37	65.0	I	3-17	I	I	I	
58	Sodium monochloroacetate	Organic salts, Halogen Compounds	3926-6																					

91	Xylene	Aromatics	1330-20-7	Wako	Liquid	0.86-0.88	3.14	7	NC	II	9	g	2018/4/3	1.8e	27	110	0.09	9.0	I
92	1,9-Decadiene	Alkenes	1647-16-1	Sigma-Aldrich	Liquid	0.76	4.28	7	NC	IV	2	g	2018/4/3	1.8e	28	>180	-0.03	0.0	NI
93	EDTA, di-potassium	Amines	25102-12-9	Sigma-Aldrich	Solid	-	-	5	NC	-	10.3	i	2018/4/3	1.8e	28	0	0.48	72.0	I
94	3-Glycidioxypropyltrimethoxysilane	Organosilicon compounds	2530-83-8	Sigma-Aldrich	Liquid	1.07	0.42	7	NC	-	2	i	2018/3/9	1.8e	28	0	0.21	21.0	I
95	iso-Octyl acrylate	Acrylates	29590-42-9	Sigma-Aldrich	Liquid	0.88	4.61	7	NC	IV	0.7	g	2018/4/3	1.8e	28	>180	-0.05	0.0	NI
96	Edhyl trimethyl acetate	Esters	3938-95-2	Sigma-Aldrich	Liquid	0.86	2.38	7	NC	III	3.8	g	2018/3/9	1.8e	27	80	0.11	14.0	I
97	2,2-Dimethyl-3-pentanol	Fatty alcohols	3970-62-5	Sigma-Aldrich	Liquid	0.83	2.27	7	NC	III	8.3	g	2018/3/9	1.8e	27	0	0.41	74.0	I
98	Betaine monohydrate	Amino acids	590-47-6	Sigma-Aldrich	Solid	-	-5.02	7	NC	-	5.3	i	2018/3/9	1.8e	27	0	0.40	32.0	I
99	Polyoxyethylene hydrogenated castorol (60E.O.)	Alkoxylated alcohols, Polymeric ethers	61788-85-0	Wako	Liquid	1.02	-	7	NC	IV	g ^f	h	2014/1/21	1.4e	26	>180	-0.01	0.0	NI
100	Dimethyl sulfoxide	Thioethers	67-68-5	Sigma-Aldrich	Liquid	1.10	-1.35	7	NC	III	7.3	i	2014/1/21	1.4e	26	>180	-0.11	0.0	NI
101	Petroleum ether	Hydrocarbons	8032-32-4	Sigma-Aldrich	Liquid	0.64	-	7	NC	-	2	i	2018/3/20	1.8e	28	>180	-0.03	0.0	NI
102	Tween80	Surfactants (nonionic)	9005-65-6	Sigma-Aldrich	Liquid	1.06-1.09	6.12	7	NC	IV	g ^f	i	2014/1/21	1.4e	26	>180	-0.02	0.0	NI
103	1,2,4-Trimethylbenzene	Hydrocarbons	95-63-6	Sigma-Aldrich	Liquid	0.88	3.63	7	NC	-	4.7	i	2014/1/21	1.4e	26	>180	-0.01	0.0	NI
104	1,2,3-Trichloropropane	Hydrocarbons	96-18-4	Sigma-Aldrich	Liquid	1.39	2.27	7	NC	III	8.7	g	2018/3/20	1.8e	28	110	0.52	36.0	I
105	1,3-Di-isopropylbenzene	Aromatics	99-62-7	Sigma-Aldrich	Liquid	0.86	4.35	7	NC	IV	2	g	2014/1/21	1.4e	26	>180	0.00	0.0	NI
106	2-(n-Dodecylthio) ethanol	Alcohol, Ether, Sulfur compound	1462-55-1	Frontier Scientific	Liquid	0.91	-	7	NC	IV	0	g	2015/3/10	1.8e	28	>180	0.00	0.0	NI
107	iso-Octylthioglycolate	Thiocompound, Ester	25103-09-7	Wako	Liquid	0.97	4.36	7	NC	IV	0.7	g	2015/3/10	1.8e	28	>180	0.00	0.0	NI
108	2,4-Difuronitrobenzene	Hydrocarbon (halogenated)	446-35-5	Wako	Liquid	1.46	-1.18	7	NC	III	4.7	g	2015/3/10	1.8e	28	60	0.11	15.6	I
109	Potassium tetrafluoroborate	Inorganic salt	14075-53-7	Sigma-Aldrich	Solid	2.51	-	7	NC	IV	0	g	2015/3/10	1.8e	28	0	0.40	19.9	I
110	Polyoxyethylene (13) (mono-, di, tri-) styrenated phenyl ether	Surfactants (nonionic)	10436-75-2	KAO	Liquid	1.12	-	7	NC	-	-	-	2018/5/29	1.8e	27	>180	-0.05	0.0	NI
111	Polyethylene (14) tribenzylated phenyl ether	Surfactants (nonionic)	16998-28-8	KAO	Liquid	1.13	-	7	NC	-	-	-	2018/5/29	1.8e	27	>180	-0.10	0.0	NI
112	Polyoxyethylene (160) sorbitan triostearate	Surfactants (nonionic)	54392-28-8	KAO	Liquid	1.07	-	7	NC	-	-	-	2018/5/29	1.8e	28	>180	-0.06	0.0	NI
113	iso-Propyl myristate	Carboxylic acid ester	110-27-0	Sigma-Aldrich	Liquid	0.85	7.71	7	NC	-	-	-	2018/5/29	1.8e	28	>180	-0.06	0.0	NI
114	Polyoxyethylene 23 lauryl ether (10%)	Surfactants (nonionic)	9002-92-0	Sigma-Aldrich	Liquid	1.02	3.54	7	NC	-	-	-	2018/6/5	1.8e	29	>180	-0.04	0.0	NI

Note -, unknown; I, GHS Category 1; 2, GHS Category 2; 2A, GHS Category 2A; 2B, GHS Category 2B; NC, not classified (United Nations, 2013); I, EPA Category I; II, EPA Category II; III, EPA Category III; IV, EPA Category IV (EPA, 1998);

*. Test was conducted in accordance with the description as previously reported in "Toxicol. Sci. 135(2): 347-355, 2013".

^a pH of 2.5(w/v)% test chemical solution

^b United Nations, 2013. Globally Harmonized System of Classification and Labeling of Chemicals (GHS), Fifth revised edition. New York and Geneva (ST/SG/AC.10/30/Rev.5).

^c EPA, 1998. Health Effects Test Guidelines OPPTS 870.2400 Acute Eye Irritation. United States Environmental Protection Agency, Washington, DC. <http://www.regulations.gov/#/documentDetail;D=EPA-HQ-OPPT-2009-0156-0006> [19 June 2015]

^d These scores were calculated from the average time-dependent profile of TEER values in three-independent experiments

^e I, irritant; NI, non-irritant

^f Data from 10% exposure condition.

^g European Centre for Ecotoxicology and Toxicology of Chemicals (ECETOC).1998. Eye irritation: reference chemicals data bank (Second Edition), ECETOC technical report No. 48. ECETOC, Brussels, Belgium.

^h Ohno Y, et al. 1999. Interlaboratory validation of the in vitro eye irritation tests for cosmetic ingredients. (1) Overview of the validation study and Draize scores for the evaluation of the tests. Toxicol. in Vitro 13, 73-98.

ⁱ Takahashi Y, et al. 2011. The Short Time Exposure (STE) test for predicting eye irritation potential: Intra-laboratory reproducibility and correspondence to globally harmonized system (GHS) and EU eye irritation classification for 109 chemicals. Toxicol. in Vitro 25, 1425-1434.