

APPENDIX V-A2

**CANDIDATE SUBSTANCES FOR THE LIST OF PROPOSED
REFERENCE SUBSTANCES FOR VALIDATION STUDIES OF
IN VITRO TEST METHODS FOR THE IDENTIFICATION OF
OCULAR CORROSIVES/SEVERE IRRITANTS
(SORTED BY GHS OCULAR HAZARD CATEGORY AND
SUBSTANCE NAME)**

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Candidate Substances (Sorted by GHS Classification and Substance Name)

GHS Classification	Substance	CASRN	In Vivo Data Source	Substance Source	Commercial Availability	Chemical Class	Product Class	Conc. Tested	Amount Tested ¹	Purity	MW	pH	Dermal Corrosivity	# of Animals Tested	Water Solubility	Log Kow	Color
Category 1	Acetic Acid	64-19-7	NIHS-Ohno	Japanese Cosmetic Industry Assn.	Sigma-Aldrich Corp.	Acid (organic) [carboxylic acid]	Industrial Chemical; Laboratory Agent, Solvent	10%	0.1 mL	n.a.	60.1	2.4	R35 (60%)	3	soluble	-0.17 (60%)	colorless
Category 1	Acid blue 40	6424-85-7	TSCA	Crompton and Knowles Corp.	Sigma-Aldrich Corp.	Amine, Quinone, Salt (organic)	Industrial Chemical	n.a.	100 mg	n.a.	473.4	8.0	noncorrosive	6	soluble (30 g/L @ 80C)	2.2	deep blue
Category 1	Methoxyethyl acrylate	3121-61-7	ECETOC	ElfAtochem, Inc.	Sigma-Aldrich Corp.	Ester, Ether	Chemical Intermediate, Industrial Chemical, Laboratory Chemical	100%	0.1 mL	99.6%	130.1	n.a.	noncorrosive	3	Soluble	0.08	?
Category 1	Aluminum chloride	16603-84-2	TSCA	Monsanto Co.	Fisher Scientific International, Inc.	Salt (inorganic)	Chemical Intermediate, Dye, Industrial Chemical, Laboratory Chemical, Pesticide, Preservative	n.a.	0.1 mL	n.a.	98.9	?	?	6	?	?	light yellow-green
Category 1	gamma-Aminopropyltriethoxy silane	919-30-2	TSCA	Union Carbide Corp.	Sigma-Aldrich Corp.	Amine, Amidine, Organosilicon Compound	Industrial Chemical	100%	0.1 mL	99%	221.4	?	R34	6	?	?	?
Category 1	Antimony oxide	1309-64-4	TSCA	Monsanto Co.	Sigma-Aldrich Corp.	Salt (inorganic)	Flame Retardant, Industrial Chemical, Laboratory Chemical, Pharmaceutical Intermediate	100%	100 mg	83.5%	291.5	?	noncorrosive	6	?	?	white powder
Category 1	Benzalkonium chloride	8001-54-5	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Onium Compound	Surfactant (cationic)	5%	0.1 mL	98%	471.5	3.1	R34 (50%)	4	soluble	n.a.	clear
Category 1	Benzalkonium chloride	8001-54-5	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Onium Compound	Surfactant (cationic)	10%	0.1 mL	98%	471.5	3.2	R34 (50%)	3	soluble	n.a.	clear
Category 1	Benzenesulfonyl chloride	98-09-9	TSCA	n.a.	Fisher Scientific International, Inc.	Acyl Halide, Sulfur Compound (organic)	Chemical Intermediate, Pesticide	n.a.	0.1 mL	99.6%	176.6	?	R34	6	?	?	brown
Category 1	Benzethonium chloride	121-54-0	LNS	n.a.	Sigma-Aldrich Corp.	Amine, Onium Compound	Anti-Infective, Pharmaceutical, Veterinary Chemical	10%	0.1 mL	n.a.	448.1	?	?	3	?	?	?
Category 1	2-Benzyl-4-chlorophenol	120-32-1	TSCA	Monsanto Co.	Sigma-Aldrich Corp.	Phenol	Anti-Fungal, Anti-Infective, Herbicide	100%	100 mg	95%	218.7	?	?	6	?	?	light brown
Category 1	2-Benzyl-4-chlorophenol	120-32-1	TSCA	Monsanto Co.	Sigma-Aldrich Corp.	Phenol	Anti-Fungal, Anti-Infective, Herbicide	n.a.	0.1 mL	n.a.	218.7	?	?	6	?	?	light brown
Category 1	2,2-Dimethyl butanoic acid	595-37-9	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Acid (organic) [carboxylic acid]	Pharmaceutical	100%	0.1 mL	96%	116.2	n.a.	R34	6	n.a.	n.a.	?
Category 1	iso-Butanol	78-83-1	ZEBET	Fisher Scientific International, Inc.	Sigma-Aldrich Corp.	Alcohol	Chemical Intermediate, Food Additive, Pesticide, Pharmaceutical Intermediate, Solvent	n.a.	0.1 mL or 100 mg	n.a.	74.1	5.7	noncorrosive	3	soluble (95 g/L)	0.76	?
Category 1	n-Butanol	71-36-3	NIHS-Ohno	Japanese Cosmetic Industry Assn.	Sigma-Aldrich Corp.	Alcohol	Chemical Intermediate, Cosmetic Ingredient, Food Additive, Industrial Chemical, Pesticide Intermediate, Pharmaceutical Intermediate, Solvent, Veterinary Chemical	10%	0.1 mL	n.a.	74.1	n.a.	noncorrosive	3	insoluble	0.88	colorless
Category 1	n-Butanol	71-36-3	ZEBET	n.a.	Sigma-Aldrich Corp.	Alcohol	Chemical Intermediate, Cosmetic Ingredient, Food Additive, Industrial Chemical, Pesticide Intermediate, Pharmaceutical Intermediate, Solvent, Veterinary Chemical	n.a.	0.1 mL or 100 mg	n.a.	74.1	?	noncorrosive	3	insoluble	0.88	colorless

GHS Classification	Substance	Physical Form Tested	MMAS score	Corneal score	Irital score	Conjunctival score	NICEATM Category 1 SubClass ²	Tested in BCOP	Tested in HET-CAM	Tested in ICE	Tested in IRE	EPA Classification	EU Classification	FHSA Classification
Category 1	Acetic Acid	liquid	68.0	n=2/3, CO=4	-	-	4	-	X	X	X	Category 1	R41	SCNM
Category 1	Acid blue 40	solid	39.7	n=2/6, CO=4	-	-	4	-	-	-	-	SCNM	R36	irritant
Category 1	Methoxyethyl acrylate	liquid	45.0	n=2/3, CO=4	-	-	4	-	-	-	-	SCNM	R36	SCNM
Category 1	Aluminum chloride	liquid	82.7	n=5/6, CO=4	-	-	4	-	-	-	-	Category 1	R41	irritant
Category 1	gamma-Aminopropyltriethoxy silane	liquid	78.7	n=5/6, CO=4	-	-	4	-	-	-	-	SCNM	Review Data	irritant
Category 1	Antimony oxide	solid	107.3	n=6/6, CO=4	n=6/6, IR=2 D14	n=6/6, CR=3, n=3/6, CC=4 D14	4	-	-	-	-	Category 1	R41	irritant
Category 1	Benzalkonium chloride	liquid	4.8	n=1/4, CO=4; n=2/4, CO=3; n=2/4, CO>0 D21	n=1/4, IR>1.5 D21	n=1/4, CR/CC>0 D21	3	X	X	X	X	Category 1	R41	SCNM
Category 1	Benzalkonium chloride	liquid	108.0	n=3/3, CO=4	n=3/3, IR=2 D21	n=1/3, CR>0, n=2/3, CC>0 D21	4	X	X	X	X	Category 1	R41	SCNM
Category 1	Benzenesulfonyl chloride	liquid	80.7	n=5/6, CO=4	-	-	4	-	-	-	-	Category 1	R41	irritant
Category 1	Benzethonium chloride	liquid	76.3	n=2/3, CO=4	-	-	4	-	-	-	-	Category 1	R41	SCNM
Category 1	2-Benzyl-4-chlorophenol	solid	100.0	n=6/6, CO=4	-	-	4	-	-	-	-	Category 1	R41	irritant
Category 1	2-Benzyl-4-chlorophenol	liquid	71.5	n=5/6, CO>0 D21	n=5/6, IR>0 D21	n=5/6, CR/CC>0 D21	1	-	-	-	-	Category 1	R41	irritant
Category 1	2,2-Dimethyl butanoic acid	liquid	44.7	n=1/6, CO=3 D14	n=1/6, IR=2 D14	-	1	X	X	X	X	Category 1	R41	irritant
Category 1	iso-Butanol	liquid	11.7	n=1/3, CO=3 D14	-	-	1	-	-	-	-	Category II	R36	SCNM
Category 1	n-Butanol	liquid	34.0	n=1/3, CO=4	-	-	4	-	X	-	-	SCNM	R41	SCNM
Category 1	n-Butanol	liquid	17.7	n=1/3, CO=4	-	-	4	-	-	-	-	SCNM	Review Data	SCNM

GHS Classification	Substance	Human Exposure Summary	Animal Exposure Summary for Category 1(H) Substances	Notes
Category 1	Acetic Acid	Has caused extreme eye and nasal irritation at concentrations in air in excess of 25 ppm. Has caused conjunctivitis at concentrations below 10 ppm. Concentrations of 200 ppm caused conjunctival hyperemia. Glacial (100%) acetic acid has caused permanent corneal opacification. A splash of vinegar (4 to 10% acetic acid solution) in the eye causes immediate pain and conjunctival hyperemia, sometimes with injury of the corneal epithelium (2 patients). Accidental application of glacial acetic acid to the eyes followed very quickly by irrigation with water resulted in immediate corneal opacification. These corneas cleared sufficiently in a few days to reveal severe iritis and small pupils fixed by posterior synechiae. Regeneration of the epithelium took many months, but corneal anesthesia and opacity were permanent. In workers exposed to aerosol concentrations of 60 ppm for 7-12 years, with daily exposures as high as 100-200 ppm, investigators found conjunctivitis (in addition to bronchitis, rharyngitis, and erosion of exposed teeth) (1, 13, 18)		
Category 1	Acid blue 40	Human data not located		
Category 1	Methoxyethyl acrylate	Human data not located		
Category 1	Aluminum chloride	Is caustic and irritating to the human eye, but in only 1 out of 55 instances of industrial corneal burns has healing been delayed beyond 2 days (10)		
Category 1	gamma-Aminopropyltriethoxy silane	Human data not located		
Category 1	Antimony oxide	Chronic exposure causes eye irritation (6, 53)		
Category 1	Benzalkonium chloride	A severe irritant to the human eye. Concentrations as low as 0.1 to 0.5% cause mild discomfort and conjunctival irritation. Slit lamp examination within 90 seconds of exposure to a single drop of 0.1% shows fine gray dots of keratitis epithelias in the corneal epithelium. Within 10 minutes of exposure, a gray haze may be seen in the corneal surface; superficial desquamation of the conjunctival epithelium may follow. These effects disappear in a day or less. (9, 17)		
Category 1	Benzalkonium chloride	A severe irritant to the human eye. Concentrations as low as 0.1 to 0.5% cause mild discomfort and conjunctival irritation. Slit lamp examination within 90 seconds of exposure to a single drop of 0.1% shows fine gray dots of keratitis epithelias in the corneal epithelium. Within 10 minutes of exposure, a gray haze may be seen in the corneal surface; superficial desquamation of the conjunctival epithelium may follow. These effects disappear in a day or less. (9, 17)		Severe effects at 5% in other study
Category 1	Benzenesulfonyl chloride	Human data not located		
Category 1	Benzethonium chloride	Human data not located		
Category 1	2-Benzyl-4-chlorophenol	Human data not located		
Category 1	2-Benzyl-4-chlorophenol	Human data not located		Tested as a solid in other study
Category 1	2,2-Dimethyl butanoic acid	Human data not located		
Category 1	iso-Butanol	Irritation of the skin, eyes, and throat have been reported from exposure to vapor or liquid. Irritation of the eyes and throat, formation of vacuoles in the superficial layers of the cornea, were reported among workers subjected to an undetermined, but apparently high concn of isobutyl alcohol & butyl acetate. (9, 20) H12		Discordant GHS classification
Category 1	n-Butanol	Is reported to cause irritation of the eyes from exposure to either vapor or liquid. Circumstantial evidence points to butyl alcohol vapor as cause of a special vacuolar keratopathy in some patients; the most severely affected it has been associated with pain & tearing, characteristically most marked on first opening eyes in morning. It can cause transient mild edema of conjunctiva of the eye. Vapor: Irritating to eyes. Considered a strong irritant of the eyes. (9, 11, 13, 27)		
Category 1	n-Butanol	Is reported to cause irritation of the eyes from exposure to either vapor or liquid. Circumstantial evidence points to butyl alcohol vapor as cause of a special vacuolar keratopathy in some patients; the most severely affected it has been associated with pain & tearing, characteristically most marked on first opening eyes in morning. It can cause transient mild edema of conjunctiva of the eye. Vapor: Irritating to eyes. Considered a strong irritant of the eyes. (9, 11, 13, 27)		Conc. tested provided in other study

GHS Classification	Substance	CASRN	In Vivo Data Source	Substance Source	Commercial Availability	Chemical Class	Product Class	Conc. Tested	Amount Tested ^a	Purity	MW	pH	Dermal Corrosivity	# of Animals Tested	Water Solubility	Log Kow	Color
Category 1	Butyl cellosolve	111-76-2	ECETOC	Fisher Scientific International, Inc.	Sigma-Aldrich Corp.	Alcohol	Solvent	100%	0.1 mL	99%	118.2	n.a.	noncorrosive	3	soluble (5 g/L)	0.83	?
Category 1	4-tert-Butylcatechol	98-29-3	TSCA	n.a.	Sigma-Aldrich Corp.	Phenol	Chemical Intermediate, Laboratory Chemical	85%	0.1 mL	n.a.	166.2	?	?	6	?	?	?
Category 1	p-tert-Butylphenol	98-54-4	TSCA	Union Carbide Corp.	Sigma-Aldrich Corp.	Phenol	Chemical Intermediate, Perfume, Pesticide	100%	80 mg	n.a.	150.2	?	?	6	?	?	?
Category 1	p-tert-Butylphenol	98-54-4	TSCA	Union Carbide Corp.	Sigma-Aldrich Corp.	Phenol	Chemical Intermediate, Perfume, Pesticide	n.a.	10 mg	n.a.	150.2	?	?	6	?	?	?
Category 1	Captan 90-concentrate (solid)	133-06-2	ECETOC	US EPA	Gustafson, LLC	Heterocyclic Compound, Sulfur Compound (organic)	Pesticide	100%	100 mg	90%	300.6	8.0	noncorrosive	3	soluble (5.1 mg/L)	2.35	white
Category 1	Cetylpyridinium bromide	140-72-7	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Onium Compound, Heterocyclic Compound	Anti-Infective; Laboratory Chemical; Surfactant (cationic)	6%	0.1 mL	99%	384.4	6.0-8.0 (0.5%)	noncorrosive	4	soluble (5 g/L)	1.83 (100%)	faintly beige
Category 1	Cetylpyridinium bromide	140-72-7	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Onium Compound, Heterocyclic Compound	Anti-Infective; Laboratory Chemical; Surfactant (cationic)	10%	0.1 mL	99%	384.4	6.0-8.0 (0.5%)	noncorrosive	6	soluble (5 g/L)	1.83 (100%)	faintly beige
Category 1	Cetyltrimethylammonium bromide	57-09-0	NIHS-Ohno	Japanese Cosmetic Industry Assn.	Sigma-Aldrich Corp.	Onium Compound, Salt (organic)	Cosmetic Ingredient	10%	0.1 mL	n.a.	364.4	5.9	noncorrosive	3	soluble (30 g/L)	3.18/2.26	?
Category 1	Chlorhexidine	55-56-1	ECETOC	n.a.	Sigma-Aldrich Corp.	Amidine	Anti-Infective, Pharmaceutical	100%	100 mg	n.a.	505.5	?	?	3	?	n.a.	?
Category 1	Cyclohexanol	108-93-0	ECETOC	Fisher Scientific International, Inc.	Sigma-Aldrich Corp.	Alcohol	Solvent	100%	0.1 mL	97%	100.2	4.5	noncorrosive	4	soluble (3.6 mg/100 mL)	1.23	colorless
Category 1	3,4-Dichlorophenyl isocyanate	102-36-3	TSCA	Mobay Corp.	Fisher Scientific International, Inc.	Isocyanate	Chemical Intermediate, Industrial Chemical	100%	0.1 mL	n.a.	188.0	?	?	3	?	?	?
Category 1	Diethylaminopropionitrile	5351-04-2	ECETOC	Elf Atochem, Inc.	Fisher Scientific International, Inc.	Amine, Nitrile	Industrial Chemical	100%	0.1 mL	>98.8 %	126.2	n.a.	noncorrosive	3	soluble	0.77	yellow
Category 1	Diethylethanolamine	100-37-8	TSCA	Union Carbide Corp.	Sigma-Aldrich Corp.	Alcohol, Amine	Chemical Intermediate, Pharmaceutical Intermediate	25%	0.1 mL	n.a.	117.2	?	?	6	?	?	colorless
Category 1	Diethylethanolamine	100-37-8	TSCA	Union Carbide Corp.	Sigma-Aldrich Corp.	Alcohol, Amine	Chemical Intermediate, Pharmaceutical Intermediate	50%	0.1 mL	n.a.	117.2	?	?	6	?	?	colorless
Category 1	Diethylethanolamine	100-37-8	TSCA	Union Carbide Corp.	Sigma-Aldrich Corp.	Alcohol, Amine	Chemical Intermediate, Pharmaceutical Intermediate	100%	0.1 mL	n.a.	117.2	?	?	6	?	?	colorless
Category 1	1,3-Diiminobenz (f)-isoindoline	65558-69-2	TSCA	Hoechst Celanese Corp.	Sigma-Aldrich Corp.	Amine, Heterocyclic Compound	Dye, Laboratory Chemical	100%	100 mg	n.a.	195.2	n.a.	?	3	?	?	?
Category 1	2,5-Dimethylhexanediol	110-03-2	ECETOC	BASF	Sigma-Aldrich Corp.	Alcohol	Chemical Intermediate	100%	40 mg	99.5%	146.2	5.7	noncorrosive	3	soluble	n.a.	?
Category 1	Bis-(3-aminopropyl) tetramethyl disiloxane	2469-55-8	TSCA	General Electric Co.	Sigma-Aldrich Corp.	Amine, Amidine, Organosilicon Compound	Industrial Chemical	100%	0.1 mL	n.a.	248.5	n.a.	R34	2	n.a.	n.a.	?
Category 1	Domiphen bromide	538-71-6	NIHS-Ohno	Japanese Cosmetic Industry Assn.	Sigma-Aldrich Corp.	Ether, Onium Compound, Salt (organic)	Anti-Infective, Pharmaceutical	10%	0.1 mL	n.a.	414.5	6.2	noncorrosive	3	n.a.	n.a.	?
Category 1	Granuform	30525-89-4	ZEBET	n.a.	Sigma-Aldrich Corp.	Aldehyde, Ether	Anti-Fungal, Anti-Infective, Industrial Chemical, Laboratory Chemical	n.a.	0.1 mL or 100 mg	n.a.	30.0	4.0	?	3	?	?	?
Category 1	Hydroxyethyl acrylate	818-61-1	TSCA	n.a.	Dow Chemical Co. (Bulk)	Alcohol, Ester	Chemical Intermediate	100%	0.1 mL	n.a.	116.1	?	?	6	?	?	?
Category 1	2-Hydroxyisobutyric acid ethylester	80-55-7	ZEBET	n.a.	Sigma-Aldrich Corp.	Alcohol, Ester	Industrial Chemical	n.a.	0.1 mL or 100 mg	n.a.	132.2	?	?	3	?	?	?
Category 1	2-Hydroxyisobutyric acid	594-61-6	ZEBET	n.a.	Sigma-Aldrich Corp.	Acid (organic) [carboxylic acid]	Industrial Chemical	n.a.	0.1 mL or 100 mg	n.a.	104.1	?	?	3	?	?	?
Category 1	HZA - Shampoo No. 7	n.a.	CTFA	Battelle Columbus Lab.	yes	Formulation	Shampoos, Hair	100%	0.1 mL	n.a.	n.a.	n.a.	n.a.	6	n.a.	n.a.	?
Category 1	HZF - Baby Shampoo No. 2	n.a.	CTFA	Battelle Columbus Lab.	yes	Formulation	Shampoos, Hair	100%	0.1 mL	n.a.	n.a.	n.a.	n.a.	6	n.a.	n.a.	n.a.
Category 1	HZI - Skin Cleanser	n.a.	CTFA	Battelle Columbus Lab.	yes	Formulation	Formulation	100%	0.1 mL	n.a.	n.a.	n.a.	n.a.	6	n.a.	n.a.	n.a.

GHS Classification	Substance	Physical Form Tested	MMAS score	Corneal score	Irital score	Conjunctival score	NICEATM Category 1 SubClass.2	Tested in BCOP	Tested in HET-CAM	Tested in ICE	Tested in IRE	EPA Classification	EU Classification	FHSA Classification
Category 1	Butyl cellosolve	liquid	68.7	-	-	n=2/3, CR>0, n=1/3, CC>0 D21	1	X	-	-	-	Category II	R36	SCNM
Category 1	4-tert-Butylcatechol	liquid	83.7	n=6/6, CO=4	n=2/6, IR=2 D21	-	4	-	-	-	-	Category I	R41	irritant
Category 1	p-tert-Butylphenol	solid	71.3	n=4/6, CO=4	-	-	4	-	-	-	-	Category I	R41	irritant
Category 1	p-tert-Butylphenol	solid	49.7	n=4/6, CO=0 D21	-	-	1	-	-	-	-	Category I	R41	irritant
Category 1	Captan 90-concentrate (solid)	solid	83.0	n=3/3, CO=4	n=1/3, IR>0 D21	n=2/3, CR/CC>0 D21	4	X	X	X	-	Category I	R41	SCNM
Category 1	Cetylpyridinium bromide	liquid	85.8	-	n=3/4, I>1.5	-	2	X	-	X	X	Category II	R36	irritant
Category 1	Cetylpyridinium bromide	liquid	89.7	n=3/6, CO=4	n=6/6, I>1.5	-	4	X	X	X	X	Category III	nonirritant	SCNM
Category 1	Cetyltrimethylammonium bromide	liquid	96.0	n=3/3, CO=4	-	n=1/3, CR=3, n=3/3, CC=2 D14	4	-	-	-	-	Category I	R41	SCNM
Category 1	Chlorhexidine	solid	82.3	n=1/3, CO=4	-	-	4	X	X	X	X	SCNM	R41	SCNM
Category 1	Cyclohexanol	liquid	79.8	n=3/4, CO=3	-	-	2	X	X	X	X	Category I	R41	SCNM
Category 1	3,4-Dichlorophenyl isocyanate	liquid	10.3	n=3/3, CO=0 D21	-	-	1	-	-	-	-	Category I	R41	SCNM
Category 1	Diethylaminopropionitrile	liquid	62.3	n=3/3, CO=4	-	-	4	-	-	-	-	Category II	R41	SCNM
Category 1	Diethylethanolamine	liquid	94.7	n=6/6, CO=4	n=3/3, IR=2 D14	-	4	-	-	-	-	Category I	R41	irritant
Category 1	Diethylethanolamine	liquid	95.0	n=6/6, CO=4	-	n=6/6, CR/CC>0 D21	4	-	-	-	-	Category I	R41	irritant
Category 1	Diethylethanolamine	liquid	82.5	n=5/6, CO=4	-	-	4	-	-	-	-	Category I	R41	irritant
Category 1	1,3-Diiminobenz (f)-isoindoline	solid	93.0	n=4/4, CO=4	-	-	4	-	-	-	-	SCNM	R41	SCNM
Category 1	2,5-Dimethylhexanediol	solid	28.3	-	n=1/3, IR = 1 D21	n=1/3, CR=2 D21	1	X	X	X	-	Category I	R41	SCNM
Category 1	Bis-(3-aminopropyl) tetramethyl disiloxane	liquid	109.0	n=2/2, CO=4	n=2/2, IR=2	n=2/2, CR=3, CC=4	4	-	-	-	-	Category I	Review Data	SCNM
Category 1	Domiphen bromide	liquid	96.3	n=3/3, CO=4	-	-	4	-	X	-	-	Category I	R41	SCNM
Category 1	Granuform	solid	75.3	n=1/3, CO=4	-	-	4	-	X	-	-	SCNM	Review Data	SCNM
Category 1	Hydroxyethyl acrylate	liquid	96.7	n=4/6, CO=4	n=6/6, IR=2 D14	-	4	-	-	-	-	Category I	R41	SCNM
Category 1	2-Hydroxyisobutyric acid ethylester	solid	81.0	n=3/3, CO=3	-	-	2	-	-	-	-	SCNM	R41	SCNM
Category 1	2-Hydroxyisobutyric acid	solid	98.7	n=3/3, CO=4	-	n=1/3, CR=3, n=3/3, CC=4	4	-	X	-	-	SCNM	R41	SCNM
Category 1	HZA - Shampoo No. 7	liquid	34.2	n=2/6, CO=1 D21	-	-	1	-	X	-	-	Category I	nonirritant	irritant
Category 1	HZF - Baby Shampoo No. 2	liquid	34.5	n=2/6, CO=1 D21	-	n=2/6, CR=2 D21	1	-	X	-	-	Category I	R41	irritant
Category 1	HZI - Skin Cleanser	liquid	37.2	n=3/6, CO=1 D21	-	-	1	-	X	-	-	Category I	R36	irritant

GHS Classification	Substance	Human Exposure Summary	Animal Exposure Summary for Category 1(H) Substances	Notes
Category 1	Butyl cellosolve	An irritant to the human eye. In several, single 8 hour exposures to concentrations of 100 to 200 ppm in air, participants reported discomfort and mild eye irritation. 7 workers exposed to aerosol concentrations of 200 to 300 ppm reported intense eye irritation, followed by recurrent ocular irritation after the initial exposure. (1, 14, 21, 24, 30)		
Category 1	4-tert-Butylcatechol	Human data not located		
Category 1	p-tert-Butylphenol	Human data not located		
Category 1	p-tert-Butylphenol	?	?	Conc. tested provided in other study
Category 1	Captan 90-concentrate (solid)	Has been reported to cause conjunctivitis (12)		
Category 1	Cetylpyridinium bromide	Human data not located		
Category 1	Cetylpyridinium bromide	Human data not located		Severe response at 6% in other study, severity based on irital effects
Category 1	Cetyltrimethylammonium bromide	In 179 patients treated with eye drops containing cetrimide (Cetyltrimethylammonium bromide) for 30 days, adverse effects were reported for 21 patients. The adverse events consisted of discomfort, blurred vision, hyperemia, burning and itching. Accidental application of cetrimide occurred during cataract surgery. This resulted in immediate corneal edema which in turn resulted in a bullous keratopathy. Four patients underwent a penetrating keratoplasty. In one patient the cornea was covered with a conjunctival flap. Light microscopy of the corneas included epithelial edema, loss of keratocytes, and a disrupted and sometimes absent endothelial cell layer. (3, 29)		
Category 1	Chlorhexidine	Acutely toxic when applied to the eye. Irreversible corneal injuries and opacification attributed to Hibiclen (chlorhexidine gluconate, a 4% topical preparation), reported in 4 female patients, aged 9 months to 83 year, in whom the drug was accidentally introduced into the eye during surgical preparation. Inadvertently used as an intraocular irrigating solution in three patients undergoing surgery. In two of the three patients, corneal endothelium damage was so severe that penetrating keratoplasty had to be performed. Further effects included pronounced iris atrophy, anterior chamber annulation, and a retrocorneal membrane. (25, 28, 31)		
Category 1	Cyclohexanol	Irritation to the eyes of human subjects results at air concentrations of 100 ppm, and which occurs after 3 to 5 minutes exposure (13, 22)		
Category 1	3,4-Dichlorophenyl isocyanate	An irritant to the human eye, causing lacrimation, and (rarely), conjunctivitis (13, 17)		
Category 1	Diethylaminopropionitrile	Human data not located		
Category 1	Diethylethanolamine	A human eye irritant (18, 42, 43)		
Category 1	Diethylethanolamine	A human eye irritant (18, 42, 43)		Severe response at 25% conc. in other study
Category 1	Diethylethanolamine	A human eye irritant (18, 42, 43)		Severe response at 25% conc. in other study
Category 1	1,3-Diiminobenz (f)-isoindoline	Human data not located		
Category 1	2,5-Dimethylhexanediol	Human data not located		
Category 1	Bis-(3-aminopropyl) tetramethyl disiloxane	Human data not located		
Category 1	Domiphen bromide	Human data not located		
Category 1	Granuform	A human eye irritant (27, 55)		
Category 1	Hydroxyethyl acrylate	Severe eye irritant (27)		
Category 1	2-Hydroxyisobutyric acid ethylester	Human data not located		
Category 1	2-Hydroxyisobutyric acid	Human data not located		
Category 1	HZA - Shampoo No. 7	?	?	Formulations excluded
Category 1	HZF - Baby Shampoo No. 2	?	?	Formulations excluded
Category 1	HZI - Skin Cleanser	?	?	Formulations excluded

GHS Classification	Substance	CASRN	In Vivo Data Source	Substance Source	Commercial Availability	Chemical Class	Product Class	Conc. Tested	Amount Tested ^a	Purity	MW	pH	Dermal Corrosivity	# of Animals Tested	Water Solubility	Log Kow	Color
Category 1	HZK - Bubble Bath	n.a.	CTFA	Battelle Columbus Lab.	yes	Formulation	Formulation	100%	0.1 mL	n.a.	n.a.	n.a.	n.a.	6	n.a.	n.a.	n.a.
Category 1	HZS - Shower Gel	n.a.	CTFA	Battelle Columbus Lab.	yes	Formulation	Formulation	100%	0.1 mL	n.a.	n.a.	n.a.	n.a.	6	n.a.	n.a.	n.a.
Category 1	HZX - Shampoo No. 2	n.a.	CTFA	Battelle Columbus Lab.	yes	Formulation	Shampoos, Hair	100%	0.1 mL	n.a.	n.a.	n.a.	n.a.	6	n.a.	n.a.	n.a.
Category 1	HZY - Anti-Dandruff Shampoo	n.a.	CTFA	Battelle Columbus Lab.	yes	Formulation	Shampoos, Hair	100%	0.1 mL	n.a.	n.a.	n.a.	n.a.	6	n.a.	n.a.	n.a.
Category 1	Imidazole	288-32-4	LNS	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Heterocyclic Compound	Anti-Fungal	20%	0.1 mL	n.a.	68.1	10.3	R34	3	soluble (633 g/L)	n.a.	?
Category 1	Imidazole	288-32-4	ECETOC	n.a.	Sigma-Aldrich Corp.	Heterocyclic Compound	Anti-Fungal	100%	100 mg	99%	68.1	10.3	R34	3	soluble (633 g/L)	n.a.	?
Category 1	Cyclohexyl isocyanate	3173-53-3	TSCA	Mobay Corp.	Sigma-Aldrich Corp.	Isocyanate	Anesthetic, Chemical Intermediate, Cleaning Agent, Industrial Chemical, Pharmaceutical Intermediate, Solvent	100%	0.1 mL	Technical Grade	125.2	n.a.	R34	2	insoluble	6.11	?
Category 1	alpha-Ketoglutaric acid alpha	328-50-7	ZEBET	n.a.	Sigma-Aldrich Corp.	Acid (organic) [carboxylic acid]	Chemical Intermediate, Laboratory Chemical, Pharmaceutical	n.a.	0.1 mL or 100 mg	n.a.	146.1	?	?	3	?	?	?
Category 1	Lactic Acid	50-21-5	NIHS-Ohno	Japanese Cosmetic Industry Assn.	Sigma-Aldrich Corp.	Alcohol, Acid (organic) [carboxylic acid]	Cosmetic Ingredient	100%	0.1 mL	n.a.	90.1	1.9	R34	3	soluble	-0.72	colorless
Category 1	Lauric acid	143-07-7	ECETOC	Unichema International, Inc.	Sigma-Aldrich Corp.	Acid (organic) [carboxylic acid]	Surfactant (anionic)	100%	52 mg	>92%	200.3	4.2	noncorrosive	3	insoluble	4.20	colorless
Category 1	4-Chloro-methanilic acid	98-36-2	ZEBET	n.a.	Fisher Scientific International, Inc.	Amine, Sulfur Compound (organic)	Chemical Intermediate, Laboratory Chemical	n.a.	0.1 mL or 100 mg	n.a.	207.6	?	?	1	?	?	?
Category 1	n-Acetyl-methionine	1115-47-5	ZEBET	n.a.	Sigma-Aldrich Corp.	Amide, Amino Acid	Cosmetic Ingredient, Food Additive, Laboratory Chemical	n.a.	0.1 mL or 100 mg	n.a.	191.3	2.2	?	3	?	?	?
Category 1	2-Methylbutyric acid	116-53-0	TSCA	Union Carbide Corp.	Sigma-Aldrich Corp.	Acid (organic) [carboxylic acid]	Chemical Intermediate, Cosmetic Ingredient, Solvent	100%	0.005 mL	97.9%	102.1	?	R34	6	?	1.18	?
Category 1	Methylpentynol	77-75-8	ZEBET	n.a.	Sigma-Aldrich Corp.	Alcohol	Pharmaceutical, Veterinary Chemical	n.a.	0.1 mL or 100 mg	n.a.	98.1	?	?	1	?	?	?
Category 1	Methylthioglycolate	2365-48-2	ECETOC	ElfaTochem, Inc.	Sigma-Aldrich Corp.	Ester, Sulfur Compound (organic)	Industrial Chemical	100%	0.1 mL	99.7%	106.1	pKa 8.22	noncorrosive	3	Soluble	0.65	?
Category 1	1-Naphthaleneacetic acid (solid)	86-87-3	ECETOC	US EPA	Sigma-Aldrich Corp.	Acid (organic) [carboxylic acid], Polycyclic Compound	Pesticide	100%	100 mg	96%	186.2	3.3	noncorrosive	6	insoluble (420 mg/L)	2.24	?
Category 1	n-Octylamine	111-86-4	TSCA	Hoechst Celanese Corp.	Sigma-Aldrich Corp.	Amine	Chemical Intermediate, Laboratory Chemical	100%	0.1 mL	n.a.	129.2	?	?	4	?	?	?
Category 1	tetra-N-Octylammonium bromide	14866-33-2	GSK	n.a.	Sigma-Aldrich Corp.	Onium Compound	Industrial Chemical, Laboratory Chemical	100%	0.1 mL or 100 mg	n.a.	546.8	?	?	1	?	?	?
Category 1	Organofunctional Silane 45-49	82985-35-1	TSCA	Union Carbide Corp.	Sigma-Aldrich Corp.	Amine, Organosilicon Compound	Polish	100%	0.005 mL	n.a.	341.6	?	?	6	?	?	?
Category 1	4-(1,1,3,3-Tetramethylbutyl)phenol	140-66-9	TSCA	Rohm and Haas Co.	Sigma-Aldrich Corp.	Phenol	Chemical Intermediate	100%	100 mg	n.a.	206.3	?	?	6	?	?	?
Category 1	Phosphorodichloridic acid, ethyl ester	1498-51-7	TSCA	Rhone-Poulenc, Inc.	Sigma-Aldrich Corp.	Ester, Organophosphorus Compound	Chemical Intermediate, Pesticide	100%	0.1 mL	96%	162.9	?	R34	6	?	?	?
Category 1	Polyethylene glycol nonylphenyl ether (Surfonic HDL-1)	9016-45-9	TSCA	Texaco, Inc.	Houghton Chemical Corp.	Alcohol, Ether	Cleaning Agent, Industrial Chemical, Pesticide, Surfactant (nonionic)	100%	0.1 mL	n.a.	308.5	?	?	6	?	?	?
Category 1	Polyethylene glycol nonylphenyl ether (Surfonic N-102)	9016-45-9	TSCA	Texaco, Inc.	Houghton Chemical Corp.	Alcohol, Ether	Cleaning Agent, Industrial Chemical, Pesticide, Surfactant (nonionic)	100%	0.1 mL	n.a.	308.5	?	?	6	?	?	?
Category 1	Polyethylene glycol nonylphenyl ether (Surfonic HDL-1)	9016-45-9	TSCA	Texaco, Inc.	Houghton Chemical Corp.	Alcohol, Ether	Cleaning Agent, Industrial Chemical, Pesticide, Surfactant (nonionic)	100%	0.1 mL	n.a.	308.5	?	?	6	?	?	?
Category 1	Potassium laurate	10124-65-9	NIHS-Ohno	Japanese Cosmetic Industry Assn.	Pfaltz & Bauer, Inc.	Acid (organic) [carboxylic acid], Salt (organic)	Cosmetic Ingredient, Pesticide	10%	0.1 mL	n.a.	238.4	?	?	3	?	?	?
Category 1	Promethazine hydrochloride	58-33-3	ECETOC	n.a.	Sigma-Aldrich Corp.	Amine, Amidine, Heterocyclic Compound, Sulfur Compound (organic)	Pharmaceutical	100%	100 mg	98%	320.9	?	?	3	n.a.	n.a.	white to faint yellow

GHS Classification	Substance	Physical Form Tested	MMAS score	Corneal score	Irital score	Conjunctival score	NICEATM Category 1 SubClass.2	Tested in BCOP	Tested in HET-CAM	Tested in ICE	Tested in IRE	EPA Classification	EU Classification	FHSA Classification
Category 1	HZK - Bubble Bath	liquid	39.7	n=5/6, CO=1 D21	-	n=3/6, CR=2 D21	1	-	X	-	-	Category I	R41	irritant
Category 1	HZS - Shower Gel	gel	39.0	n=2/6, CO>1 D21	-	n=2/6, CR=2 D21	1	-	X	-	-	Category I	R41	irritant
Category 1	HZX - Shampoo No. 2	liquid	39.3	n=2/6, CO=1 D21	-	-	1	-	X	-	-	Category I	R36	irritant
Category 1	HZY - Anti-Dandruff Shampoo	liquid	37.2	n=2/6, CO=1 D21	-	-	1	-	X	-	-	Category I	R41	irritant
Category 1	Imidazole	liquid	48.7	n=1/3, CO=3 D14	-	-	1	-	-	-	-	Category I	R41	SCNM
Category 1	Imidazole	solid	59.3	n=2/3, CO=4	n=2/3, I>1.5	-	4	X	X	X	X	Category I	R41	SCNM
Category 1	Cyclohexyl isocyanate	liquid	101.0	n=2/2, CO=4	-	-	4	-	-	X	-	Category I	R41	SCNM
Category 1	alpha-Ketoglutaric acid alpha	solid	93.0	n=2/3, CO=4	-	-	4	-	-	-	-	SCNM	R41	SCNM
Category 1	Lactic Acid	liquid	102.7	n=3/3, CO=4	-	n=3/3, CR/CC=2 D14	4	-	X	-	-	Category I	R41	SCNM
Category 1	Lauric acid	solid	38.0	n=3/3, CO>1 D21	-	n=3/3, CR=1 D21	1	-	-	-	-	Category I	R41	SCNM
Category 1	4-Chloro-methanilic acid	solid	17.0	n=1/1, CO=4	-	-	4	-	-	-	-	SCNM	Review Data	SCNM
Category 1	n-Acetyl-methionine	solid	57.3	n=1/3, CO=4	-	-	4	-	X	-	-	SCNM	R41	SCNM
Category 1	2-Methylbutyric acid	liquid	38.3	n=2/6, CO=4	-	-	4	-	-	-	-	Category I	Review Data	SCNM
Category 1	Methylpentynol	liquid	34.0	n=1/1, CO=4	-	-	4	-	X	-	-	Category I	R41	SCNM
Category 1	Methylthioglycolate	liquid	53.0	n=1/3, CO=4	-	-	4	-	-	-	-	Category II	R36	SCNM
Category 1	1-Naphthaleneacetic acid (solid)	solid	46.7	n=1/6, CO=4	-	-	4	X	X	X	-	Category I	R41	irritant
Category 1	n-Octylamine	liquid	79.5	n=4/4, CO=4	-	-	4	-	-	-	-	Category I	R41	SCNM
Category 1	tetra-N-Octylammonium bromide	solid	0.0	-	-	-	0 (likely 4)	-	-	-	X	Category I	R41	SCNM
Category 1	Organofunctional Silane 45-49	liquid	54.2	n=2/6, CO>0 D21	n=2/6, IR>0 D21	n=2/6, CR>0 D21	1	-	-	-	-	Category I	R41	SCNM
Category 1	4-(1,1,3,3-Tetramethylbutyl)phenol	solid	90.0	n=6/6, CO=3	n=6/6, IR=2	-	2	-	-	-	-	SCNM	R41	SCNM
Category 1	Phosphorodichloridic acid, ethyl ester	liquid	100.0	n=6/6, CO=4	-	n=6/6, CR=3, CC=4 D21	4	-	-	-	-	Category I	R41	irritant
Category 1	Polyethylene glycol nonylphenyl ether (Surfonic HDL-1)	liquid	35.0	-	-	-	0	-	-	-	-	SCNM	Review Data	irritant
Category 1	Polyethylene glycol nonylphenyl ether (Surfonic N-102)	liquid	38.3	n=2/6, CO=4	-	-	4	-	-	-	-	Category I	R41	irritant
Category 1	Polyethylene glycol nonylphenyl ether (Surfonic HDL-1)	liquid	52.3	n=5/6, CO=4	-	-	4	-	-	-	-	Category I	R41	irritant
Category 1	Potassium laurate	liquid	33.7	n=1/3, CO=4 D14	-	-	4	-	-	-	-	Category I	R41	SCNM
Category 1	Promethazine hydrochloride	solid	71.7	n=3/3, CO=3	n=3/3, IR=2	-	3	X	X	X	X	Category I	R41	SCNM

GHS Classification	Substance	Human Exposure Summary	Animal Exposure Summary for Category 1(H) Substances	Notes
Category 1	HZK - Bubble Bath	?	?	Formulations excluded
Category 1	HZS - Shower Gel	?	?	Formulations excluded
Category 1	HZX - Shampoo No. 2	?	?	Formulations excluded
Category 1	HZY - Anti-Dandruff Shampoo	?	?	Formulations excluded
Category 1	Imidazole	Human data not located		Tested as a solid in other study
Category 1	Imidazole	Human data not located		
Category 1	Cyclohexyl isocyanate	Human data not located		
Category 1	alpha-Ketoglutaric acid alpha	Human data not located		
Category 1	Lactic Acid	Effect on the eye is similar to that of other acids of moderate strength, causing initial epithelial coagulation on the cornea and conjunctiva; more concentrated solutions can cause severe burns of the skin or eye (10, 20)		
Category 1	Lauric acid	Human data not located		
Category 1	4-Chloro-methanilic acid	Human data not located		
Category 1	n-Acetyl-methionine	Human data not located		
Category 1	2-Methylbutyric acid	Human data not located		
Category 1	Methylpentynol	Human data not located		
Category 1	Methylthioglycolate	Human data not located		
Category 1	1-Naphthaleneacetic acid (solid)	Has been reported to cause severe irritation to the human eye (17)		
Category 1	n-Octylamine	Human data not located		
Category 1	tetra-N-Octylammonium bromide	Human data not located		
Category 1	Organofunctional Silane 45-49	Human data not located		
Category 1	4-(1,1,3,3-Tetramethylbutyl)phenol	A human eye irritant (23)		
Category 1	Phosphorodichloridic acid, ethyl ester	Vapor causes eye irritation; liquid causes severe burns to eye (27)		
Category 1	Polyethylene glycol nonylphenyl ether (Surfonic HDL-1)	?	?	Used study demonstrating most consistent animal responses
Category 1	Polyethylene glycol nonylphenyl ether (Surfonic N-102)	Human data not located		Used study demonstrating most consistent animal responses
Category 1	Polyethylene glycol nonylphenyl ether (Surfonic HDL-1)	Human data not located		
Category 1	Potassium laurate	Human data not located		
Category 1	Promethazine hydrochloride	Severe eye irritant (17)		

GHS Classification	Substance	CASRN	In Vivo Data Source	Substance Source	Commercial Availability	Chemical Class	Product Class	Conc. Tested	Amount Tested ¹	Purity	MW	pH	Dermal Corrosivity	# of Animals Tested	Water Solubility	Log Kow	Color
Category 1	Promethazine hydrochloride	58-33-3	LNS	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Amine, Amidine, Heterocyclic Compound, Sulfur Compound (organic)	Pharmaceutical	20%	0.1 mL	n.a.	320.9	4.5	noncorrosive	3	n.a.	n.a.	white to faint yellow
Category 1	Protectol PP	80-54-6	TSCA	BASF	Sigma-Aldrich Corp.	Aldehyde	Food Additive, Perfume	100%	0.1 mL	84.8%	204.3	n.a.	noncorrosive	3	n.a.	?	white powder
Category 1	Pyridine	110-86-1	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Heterocyclic Compound	Pesticide Intermediate, Pharmaceutical Intermediate, Solvent	100%	0.1 mL	99.9+%	79.1	9.9	noncorrosive	3	soluble	0.65	?
Category 1	Quinacrine	69-05-6	LNS	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Amine, Heterocyclic Compound, Polycyclic Compound	Pharmaceutical	20%	0.1 mL	n.a.	472.9	3.8	noncorrosive	3	soluble (1 g/36 mL)	n.a.	?
Category 1	Quinacrine	69-05-6	ECETOC	n.a.	Sigma-Aldrich Corp.	Amine, Heterocyclic Compound, Polycyclic Compound	Pharmaceutical	100%	100 mg	90%	472.9	?	noncorrosive	3	soluble (1 g/36 mL)	n.a.	?
Category 1	beta-Resorcylic acid	89-86-1	ZEBET	n.a.	Sigma-Aldrich Corp.	Acid (organic) [carboxylic acid], Phenol	Chemical Intermediate, Dye	n.a.	0.1 mL or 100 mg	n.a.	154.1	?	?	1	?	?	?
Category 1	Sodium hydrogen sulfate	7681-38-1	ZEBET	n.a.	Sigma-Aldrich Corp.	Salt (inorganic)	Cleaning Agent, Laboratory Chemical, Pesticide	n.a.	0.1 mL or 100 mg	n.a.	120.1	?	?	1	?	?	?
Category 1	Sodium hydroxide	1310-73-2	ECETOC	Fisher Scientific International, Inc.	Sigma-Aldrich Corp.	Alkali	Caustic Agent, Chemical Intermediate, Industrial Chemical, Pharmaceutical Intermediate, Veterinary Chemical	10%	0.1 mL	Reagent Grade	40.0	12.7	R35 (5%)	1	soluble (1 g/0.9 mL)	"virtually 0"	?
Category 1	Sodium oxalate	62-76-0	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Acid (organic) [carboxylic acid]	Industrial Chemical, Laboratory Chemical	100%	100 mg	>99%	134.0	9.4	corrosive	3	soluble (37 g/L)	n.a.	?
Category 1	Sodium perborate tetrahydrate	10486-00-7	ECETOC	Dupont Corp.	Sigma-Aldrich Corp.	Boron Compound, Salt (inorganic)	Cleaning Agent	100%	60 mg	98.6%	153.9	10.0	noncorrosive	6	n.a.	n.a.	?
Category 1	Di(2-ethylhexyl) sodium sulfosuccinate	98-09-9	NIHS-Ohno	Japanese Cosmetic Industry Assn.	Sigma-Aldrich Corp.	Ester, Salt (organic), Sulfur Compound (organic)	Adjuvant, Cleaner, Solubilizer, Wetting Agent	10%	0.1 mL	n.a.	444.6	6.5	noncorrosive	3	soluble (15 g/L)	n.a.	?
Category 1	Dibenzoyl-L-tartaric acid	2743-38-6	LNS	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Acid (organic) [carboxylic acid], Ester	Chemical Intermediate	20%	0.1 mL	n.a.	358.3	2.4	noncorrosive	3	slightly soluble	n.a.	?
Category 1	Dibenzoyl-L-tartaric acid	2743-38-6	ECETOC	n.a.	Sigma-Aldrich Corp.	Acid (organic) [carboxylic acid], Ester	Chemical Intermediate	100%	100 mg	98%	358.3	n.a.	noncorrosive	3	slightly soluble	n.a.	?
Category 1	Tetraethylene glycol diacrylate	17831-71-9	TSCA	Rhone-Poulenc, Inc.	Sigma-Aldrich Corp.	Ether, Nitro Compound	Chemical Intermediate, Industrial Chemical	100%	0.1 mL	n.a.	302.3	?	?	6	?	?	?
Category 1	Tetrahydrofuran	109-99-9	TSCA	International Specialty Products Co.	Sigma-Aldrich Corp.	Ether, Heterocyclic Compound	Chemical Intermediate, Industrial Chemical, Pharmaceutical Intermediate, Solvent	100%	0.1 mL	n.a.	72.1	?	?	6	?	?	?
Category 1	N,N,N',N'-Tetramethylhexanediamine	111-18-2	TSCA	Union Carbide Corp.	Sigma-Aldrich Corp.	Amine	Anti-Infective, Industrial Chemical, Laboratory Chemical	100%	0.005 mL	n.a.	172.3	?	?	6	?	?	?
Category 1	2-Nitro-4-thiocyananiline	54029-45-7	GSK	n.a.	Sigma-Aldrich Corp.	Amine, Nitro Compound, Sulfur Compound (organic)	Industrial Chemical	100%	0.1 mL or 100 mg	n.a.	195.2	?	?	1	?	?	?
Category 1	TNO-35 (Propyl lactate)	616-09-1	TNO-Prinsen	n.a.	Cook Aromatics Ltd. (Bulk)	Alcohol, Ester	Cleaning Agent, Food Additive	n.a.	0.1 mL or 100 mg	n.a.	132.2	?	?	1	?	?	?
Category 1	1,2,4-Triazole, sodium salt	41253-21-8	ECETOC	Elf Atochem, Inc.	Sigma-Aldrich Corp.	Heterocyclic Compound, Salt (organic)	Anti-Fungal	100%	100 mg	99%	91.1	n.a.	noncorrosive	1	soluble	n.a.	brown
Category 1	Trichloroacetic acid	76-03-9	ECETOC	Fisher Scientific International, Inc.	Sigma-Aldrich Corp.	Acid (organic) [carboxylic acid]	Caustic Agent, Herbicide	30%	0.1 mL	Reagent Grade	163.4	0.7	R34 (0.6N); R35 (undiluted)	1	soluble (10 g/mL)	1.33	?
Category 1	Trichloroacetyl chloride	76-02-8	TSCA	Rhone-Poulenc, Inc.	Sigma-Aldrich Corp.	Acyl Halide	Chemical Intermediate, Industrial Chemical	n.a.	0.1 mL	n.a.	163.4	?	?	4	?	?	?
Category 1	Triton X-100	9002-93-1	ECETOC	Union Carbide Corp.	Sigma-Aldrich Corp.	Ether	Surfactant (nonionic)	10%	0.1 mL	98%	250.4	n.a.	noncorrosive	6	soluble	n.a.	colorless
Category 1	Triton X-100	9002-93-1	TSCA	Union Carbide Corp.	Sigma-Aldrich Corp.	Ether	Surfactant (nonionic)	100%	0.1 mL	n.a.	250.4	n.a.	noncorrosive	6	soluble	n.a.	colorless
Category 1	Triton X-100	9002-93-1	NIHS-Ohno	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Ether	Surfactant (nonionic)	100%	0.1 mL	n.a.	250.4	6.8	noncorrosive	3	soluble	n.a.	colorless
Category 1	Triton X-100	9002-93-1	TSCA	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Ether	Surfactant (nonionic)	100%	100 mg	n.a.	250.4	9.7 (100%)	noncorrosive	6	soluble	n.a.	colorless

GHS Classification	Substance	Physical Form Tested	MMAS score	Corneal score	Irital score	Conjunctival score	NICEATM Category 1 SubClass.2	Tested in BCOP	Tested in HET-CAM	Tested in ICE	Tested in IRE	EPA Classification	EU Classification	FHSA Classification
Category 1	Promethazine hydrochloride	liquid	84.0	n=3/3, CO=4	-	-	4	-	-	-	-	Category I	R41	SCNM
Category 1	Protectol PP	liquid	34.3	n=2/3, CO=0 D21	-	n=3/3, CR=0 D21	1	-	-	-	-	Category I	R41	SCNM
Category 1	Pyridine	liquid	48.0	n=1/3, CO=4	n=1/3, IR=2 D14	-	4	X	X	X	-	Category I	R41	SCNM
Category 1	Quinacrine	liquid	52.3	n=1/3, CO=4	n=3/3, IR=2 D14	-	1	-	-	-	-	Category I	R41	SCNM
Category 1	Quinacrine	solid	82.0	n=3/3, CO=3	n=3/3, IR=2	-	3	X	X	X	-	Category I	R41	SCNM
Category 1	beta-Resorcylic acid	solid	63.0	n=1/1, CO=4	-	-	4	-	-	-	-	SCNM	Review Data	SCNM
Category 1	Sodium hydrogen sulfate	solid	8.0	n=1/1, CO=4	-	-	4	-	-	-	-	SCNM	Review Data	SCNM
Category 1	Sodium hydroxide	liquid	108.0	n=1/1, CO=4	n=1/1, IR=2 D21	n=1/1, CR/CC=3 D21	4	X	X	X	X	Category I	R41	SCNM
Category 1	Sodium oxalate	solid	61.3	n=1/3, CO=4	n=1/3, IR=2 D14	-	4	X	X	X	-	Category I	R41	SCNM
Category 1	Sodium perborate tetrahydrate	solid	30.5	n=4/6, CO>1 D21	-	-	1	X	X	X	-	Category I	R41	SCNM
Category 1	Di(2-ethylhexyl) sodium sulfosuccinate	liquid	57.0	n=1/3, CO=4	-	-	4	-	-	-	-	SCNM	R41	SCNM
Category 1	Dibenzoyl-L-tartaric acid	liquid	33.7	n=2/3, CO=4	-	-	4	-	-	X	-	SCNM	R41	SCNM
Category 1	Dibenzoyl-L-tartaric acid	solid	36.7	n=3/3, CO=3	-	-	3	X	X	X	-	Category I	R41	SCNM
Category 1	Tetraethylene glycol diacrylate	liquid	103.3	n=5/6, CO=4	n=6/6, IR=2 D14	-	4	-	-	-	-	Category I	R41	irritant
Category 1	Tetrahydrofuran	liquid	31.2	n=2/6, CO=4	-	-	4	-	-	-	-	SCNM	Review Data	irritant
Category 1	N,N,N',N'-Tetramethylhexanediamine	liquid	96.0	n=6/6, CO=4	-	-	4	-	-	-	-	Category I	R41	irritant
Category 1	2-Nitro-4-thiocyananiline	solid	63.0	-	-	-	0 (likely 4)	-	-	-	X	Category I	R41	SCNM
Category 1	TNO-35 (Propyl lactate)	solid	63.0	n=1/1, CO>0 D21	n=1/1, IR>0 D21	n=1/1, CC>0 D21	1	-	-	X	-	Category I	R41	SCNM
Category 1	1,2,4-Triazole, sodium salt	solid	104.0	n=1/1, CO=4	n=1/1, IR=2	-	4	-	-	-	-	Category I	R41	SCNM
Category 1	Trichloroacetic acid	liquid	106.0	n=1/1, CO=4	n=1/1, IR=2 D21	n=1/1, CR/CC=2 D21	4	X	X	X	X	Category I	R41	SCNM
Category 1	Trichloroacetyl chloride	liquid	91.0	n=4/4, CO=4	-	-	4	-	-	-	-	Category I	R41	SCNM
Category 1	Triton X-100	liquid	68.7	-	n=2/6, IR>1.5	n=1/6, CR=0	3	X	X	X	X	SCNM	R41	irritant
Category 1	Triton X-100	liquid	65.8	n=2/6, CO=4	-	-	4	-	-	-	-	SCNM	Review Data	irritant
Category 1	Triton X-100	liquid	41.3	n=1/3, CO=3 D14	-	-	1	-	-	-	-	Category III	nonirritant	irritant
Category 1	Triton X-100	solid	51.7	-	n=5/6, IR>1.5	-	2	-	-	-	-	Category III	nonirritant	SCNM

GHS Classification	Substance	Human Exposure Summary	Animal Exposure Summary for Category 1(H) Substances	Notes
Category 1	Promethazine hydrochloride	Severe eye irritant (17)		ECETOC study noted irital effects when tested at 100% as a solid
Category 1	Protectol PP	Severe eye irritant (17)		
Category 1	Pyridine	Causes irritation upon contact with the eyes (6, 20)		
Category 1	Quinacrine	Direct contact with the eye causes yellow staining of the bulbar conjunctiva and cornea; in more severe reactions striate keratopathy or wrinkling of the posterior surface of cornea develops, presumably due to corneal edema (11)		In ECETOC study, tested at 100% as a solid
Category 1	Quinacrine	Direct contact with the eye causes yellow staining of the bulbar conjunctiva and cornea; in more severe reactions striate keratopathy or wrinkling of the posterior surface of cornea develops, presumably due to corneal edema (11)		
Category 1	beta-Resorcylic acid	Human data not located		
Category 1	Sodium hydrogen sulfate	Human data not located		
Category 1	Sodium hydroxide	Contact with the eyes causes disintegration and sloughing of conjunctival and corneal epithelia, corneal opacification, marked edema, and ulceration; after 7 to 13 days either gradual recovery begins, or there is progression of ulceration and corneal opacification. Opacification may be so severe that iris markings are not discernable. Complications of severe eye burns are symblepharon, with overgrowth of the cornea by a vascularized membrane, progressive or recurrent corneal ulceration, permanent corneal opacification, necrosis of the bulbar conjunctiva, blanching and necrotic corneal cul-de-sac, and blindness. Eye contact: Levels of toxic effect: (1) Irritation. (2) Conjunctivitis, corneal burns. (3) Photophobia. (4) Disintegration and sloughing of conjunctival and corneal epithelium. (5) Corneal edema, ulceration, and opacification. (6) Symblepharon. (7) Overgrowth of the cornea by a vascularized membrane. (8) Permanent corneal opacification. (11, 18)		
Category 1	Sodium oxalate	Human data not located		
Category 1	Sodium perborate tetrahydrate	Very few cases of eye irritation were observed (26)		
Category 1	Di(2-ethylhexyl) sodium sulfosuccinate	In ophthalmological formulations, concentrations of greater than 0.1% may cause conjunctival irritation; repeated use of such drugs may delay healing of corneal lesions. (7)		
Category 1	Dibenzoyl-L-tartaric acid	Human data not located		Tested as a solid in other study
Category 1	Dibenzoyl-L-tartaric acid	Human data not located		
Category 1	Tetraethylene glycol diacrylate	Human data not located		
Category 1	Tetrahydrofuran	A human eye irritant (27)		
Category 1	N,N,N',N'-Tetramethylhexanediamine	Human data not located		
Category 1	2-Nitro-4-thiocyananiline	Human data not located		
Category 1	TNO-35 (Propyl lactate)	Human data not located		
Category 1	1,2,4-Triazole, sodium salt	Human data not located		
Category 1	Trichloroacetic acid	Reported to be irritating and very painful to the human eye (15, 19)		
Category 1	Trichloroacetyl chloride	Reported to be irritating and very painful to the human eye (15, 19)		
Category 1	Triton X-100	Human data not located		Decided to use Triton X-100 at different conc.; this was maximum concentration tested
Category 1	Triton X-100	Human data not located		
Category 1	Triton X-100	?	?	
Category 1	Triton X-100	Human data not located		All other concn. tested as a liquid; excluded to be consistent

GHS Classification	Substance	CASRN	In Vivo Data Source	Substance Source	Commercial Availability	Chemical Class	Product Class	Conc. Tested	Amount Tested ¹	Purity	MW	pH	Dermal Corrosivity	# of Animals Tested	Water Solubility	Log Kow	Color
Category 1(H)	Ammonia	7664-41-7	-	-	Sigma-Aldrich Corp.	Alkali	Anti-Fungal, Chemical Intermediate, Cleaning Agent, Fertilizer, Herbicide, Industrial Chemical, Refrigerant	-	-	-	17.0	-	-	-	n.a.	n.a.	?
Category 1(H)	Chloroform	67-66-3	-	n.a.	Sigma-Aldrich Corp.	Hydrocarbon (acyclic)	Anesthetic, Chemical Intermediate, Cleaning Agent, Industrial Chemical, Pharmaceutical Intermediate, Solvent	-	-	-	119.4	-	-	-	n.a.	n.a.	?
Category 1(H)	Lime	1305-78-8	-	-	Sigma-Aldrich Corp.	Salt (inorganic)	Building Material, Chemical Intermediate, Cleaning Agent, Fertilizer, Industrial Chemical	-	-	-	56.1	-	-	-	n.a.	n.a.	white to grayish
Category 1(H)	Magnesium hydroxide	12141-11-6	-	-	Sigma-Aldrich Corp.	Salt (inorganic)	Chemical Intermediate, Flame Retardant, Industrial Chemical, Pharmaceutical, Veterinary Agent	-	-	-	42.3	-	-	-	n.a.	n.a.	?
Category 1(H)	Nitric acid	7697-37-2	-	-	Sigma-Aldrich Corp.	Acid, Salt (inorganic)	Chemical Intermediate, Industrial Chemical, Laboratory Reagent, Pharmaceutical Intermediate	-	-	-	63.0	-	-	-	n.a.	n.a.	colorless to yellow
Category 1(H)	Potassium hydroxide	1310-58-3	-	-	Sigma-Aldrich Corp.	Alkali, Salt (inorganic)	Chemical Intermediate, Cleaning Agent, Fertilizer, Food Additive, Industrial Chemical, Veterinary Chemical	-	-	-	56.1	-	-	-	n.a.	n.a.	?
Category 1(H)	Silver nitrate	7761-88-8	-	-	Sigma-Aldrich Corp.	Nitrate, Salt (inorganic)	Anti-Infective, Chemical Intermediate, Dye, Industrial Chemical, Laboratory Chemical, Pharmaceutical, Pharmaceutical Intermediate	-	-	-	169.9	-	-	-	n.a.	n.a.	white to grayish-black
Category 1(H)	Sodium hydrogen difluoride	1333-83-1	-	-	Sigma-Aldrich Corp.	Salt (inorganic)	Anti-Infective, Cleaning Agent, Industrial Chemical, Preservative	-	-	-	62.0	-	-	-	n.a.	n.a.	?
Category 1(H)	Sulfuric acid	7664-93-9	-	-	Sigma-Aldrich Corp.	Acid (inorganic), Sulfur Compound (inorganic)	Battery Acid, Chemical Intermediate, Cleaning Agent, Fertilizer, Food Additive, Industrial Chemical, Laboratory Chemical	-	-	-	98.1	-	-	-	n.a.	n.a.	?
Category 1(H)	Zinc chloride	7646-85-7	-	-	Sigma-Aldrich Corp.	Salt (inorganic)	Anti-Infective, Flame Retardant, Herbicide, Industrial Chemical, Pesticide, Preservative	-	-	-	136.3	-	-	-	n.a.	n.a.	?
Category 2A	Methyl acetate	79-20-9	ECETOC	Fisher Scientific International, Inc.	Sigma-Aldrich Corp.	Ester	Chemical Intermediate, Food Additive, Herbicide, Laboratory Chemical, Solvent	100%	0.1 mL	98%	74.1	n.a.	?	4	243 g/L	0.18	colorless

GHS Classification	Substance	Physical Form Tested	MMAS score	Corneal score	Irital score	Conjunctival score	NICEATM Category 1 SubClass.2	Tested in BCOP	Tested in HET-CAM	Tested in ICE	Tested in IRE	EPA Classification	EU Classification	FHSA Classification
Category 1(H)	Ammonia	Liquid	-	-	-	-	-	-	-	-	-	-	-	-
Category 1(H)	Chloroform	liquid	-	-	-	-	-	-	-	-	-	-	-	-
Category 1(H)	Lime	solid	-	-	-	-	-	-	-	-	-	-	-	-
Category 1(H)	Magnesium hydroxide	solid	-	-	-	-	-	-	-	-	-	-	-	-
Category 1(H)	Nitric acid	liquid	-	-	-	-	-	-	-	-	-	-	-	-
Category 1(H)	Potassium hydroxide	solid	-	-	-	-	-	-	-	-	-	-	-	-
Category 1(H)	Silver nitrate	liquid	-	-	-	-	-	-	-	-	-	-	-	-
Category 1(H)	Sodium hydrogen difluoride	liquid	-	-	-	-	-	-	-	-	-	-	-	-
Category 1(H)	Sulfuric acid	liquid	-	-	-	-	-	-	-	-	-	-	-	-
Category 1(H)	Zinc chloride	solid	-	-	-	-	-	-	-	-	-	-	-	-
Category 2A	Methyl acetate	liquid	39.5	-	-	-	-	X	X	X	X	Category II	R36	SCNM

GHS Classification	Substance	Human Exposure Summary	Animal Exposure Summary for Category 1(H) Substances	Notes
Category 1(H)	Ammonia	Ammonia vapors cause irritation of eyes, with high concentrations causing conjunctivitis. Corneal edema and semi-dilated, fixed pupils are typical. Ammonia has a greater tendency than other alkalis to penetrate and damage the iris, and to cause cataract. In severe burns, iritis may be accompanied by hypopyon or hemorrhages, extensive loss of pigment and severe glaucoma. Exposure to high gas concentrations of ammonia may cause temporary blindness and severe eye damage. Direct contact of the eyes with liquid anhydrous ammonia will produce serious eye burns. 2 cases of ocular injuries with a rise in intraocular pressure and cataract formation after ammonia of unknown concentration had been squirted into the victims' eyes during robberies were reported. In both cases, the more severely affected eyes showed marked injection and edema of the conjunctiva; diffuse corneal damage; semi-dilated, oval, and fixed pupils; and a marked increase of the intraocular pressure, which persisted and was controlled only with drugs. Glaucoma was observed to be associated with an open angle.	Corneal opacity was observed in rabbits following continuous exposure to ammonia vapor (470 mg/M3). Swine exposed to ammonia for 2 to 6 weeks at 100 PPM in air developed conjunctival irritation. Continuous exposure of rabbits to 470 mg/cu m for several weeks produced opacities over ¼ to ½ of the cornea. Even fairly low airborne concentrations of ammonia produce rapid eye and nose irritation. Contact with concentrated ammonia solutions, such as some industrial cleaners, can cause serious corrosive injury (6, 11, 56).	
Category 1(H)	Chloroform	Splash of liquid chloroform in the eyes causes immediate burning pain, tearing and reddening of the conjunctiva. The corneal epithelium is usually injured and partially lost. Exposure to liquid or gaseous chloroform causes keratitis, corneal opacities, and ulceration (11, 37, 38, 39, 40, 41)	Liquid chloroform produced slight injury to the eyes which took over a week to heal. (62)	
Category 1(H)	Lime	The major complaints of workers exposed to lime consist of eye and skin irritation. Calcium oxide dust irritates the eyes primarily because of its alkalinity. Exposure to lime has been reported to cause conjunctival necrosis, symblepharon, keratitis, corneal necrosis, corneal opacities, corneal scarring, corneal ulceration, corneal vascularization and iritis (1,5,44)	Animal Data Not Located	
Category 1(H)	Magnesium hydroxide	Human ocular exposure to magnesium hydroxide produces combined thermal and alkali injury. Reported effects of exposure to magnesium hydroxide are conjunctival necrosis, symblepharon, keratitis, corneal necrosis, corneal opacities, corneal scarring, corneal ulceration, corneal vascularization and iritis (44, 45)	Milk of magnesia applied to rabbit eyes twice a day for three or four days caused damage to the corneal epithelium, demonstrable by staining with fluorescein. After the applications were discontinued, the corneas returned to normal in two or three days. (10)	
Category 1(H)	Nitric acid	Contact of nitric acid with the eye causes immediate opacification of the corneal and conjunctival epithelium. It also causes symblepharon, shrinkage of the globe, keratitis, corneal ulceration and corneal and conjunctival necrosis (11, 17, 46)	Animal Data Not Located	
Category 1(H)	Potassium hydroxide	Eye contact with concentrated alkalis such as potassium hydroxide causes conjunctival edema and corneal destruction. Potassium hydroxide (caustic potash) is one of the strongest alkalis. It is extremely corrosive, and many reports have been made of devastating damage of the eye from contact with either the solid or solutions of potassium hydroxide. The type of injury is essentially the same as that produced by sodium hydroxide and other strong alkalis, and includes iritis, conjunctival necrosis, symblepharon, keratitis, corneal necrosis, opacities, scarring, ulceration and vascularization (1, 11, 27, 45, 47)	Animal Data Not Located	
Category 1(H)	Silver nitrate	Solid silver nitrate, known as lunar caustic, can be very injurious to the eye. Particles of solid silver nitrate in the conjunctival sac have been known to cause severe inflammation with deep injury to surrounding tissues, scarring, and symblepharon. In a most unusual case of severe injury from solid nitrate the cornea became dark brown, and the lens became cataractous. Concentration solutions of silver nitrate from 5%-50% applied by mistake or accidentally splashed in the eye have caused severe injury, with permanent corneal opacification in some cases. Solutions of high concentration cause rapid appearance of edema of the conjunctiva and lids, with bloody purulent discharge from the conjunctival sac. Opacification of the cornea may result and may be permanent (5, 11, 13, 48, 49, 50)	Treatment of rat eyes with a single 3-drops 0.66% silver nitrate soln caused deposition of silver in the cornea, conjunctiva, subconjunctiva, Bowman's layer, reticular fibers of the corneal stroma, Descemet's membrane and the posterior corneal epithelium. Morphologic evolution of the early events of corneal vascularization in the rat cornea induced by silver nitrate cautery was followed by light and electron microscopy. An initial acute inflammatory response occurred within the first 6 hours after cautery as evidenced by vascular dilation, diapedesis of leukocytes, and an increased vascular permeability, as manifested by distended lymphatics and the presence of extravascular fibrin. At 33 hours after cautery, the first new vessels were observed as sprouts from the capillary arcade and postcapillary venules. Adult male Sprague-Dawley rats were anesthetized with halothane gas, and the centers of their right corneas treated with a silver nitrate applicator stick (75% silver nitrate, 25% potassium nitrate) to produce a discrete lesion. This substance causes the formation of hydrofluoric acid when exposed to mucous membranes. Ocular toxicity is caused by hydrofluoric acid. In inhalation studies in rabbits and guinea pigs, a concentration of 50 MG/CU M, hydrogen fluoride induced discharge from the eyes. Experimental splash burns of hydrofluoric acid into the eyes of rabbits have shown a 20% solution to cause immediate damage with total corneal opacification with conjunctival ischemia, and with corneal stromal edema within an hour, followed by necrosis of anterior ocular structures. An 8% solution produced ischemia and corneal stromal edema persisting for 40-65 days, accompanied by corneal vascularization. Even a 2% solution caused mild persistent stromal edema and vascularization. (6, 11)	
Category 1(H)	Sodium hydrogen difluoride	Exposure to concentrated sodium hydrogen difluoride has caused corneal necrosis, opacification, scarring, ulceration, vascularization (11, 23)	This substance causes the formation of hydrofluoric acid when exposed to mucous membranes. Ocular toxicity is caused by hydrofluoric acid. In inhalation studies in rabbits and guinea pigs, a concentration of 50 MG/CU M, hydrogen fluoride induced discharge from the eyes. Experimental splash burns of hydrofluoric acid into the eyes of rabbits have shown a 20% solution to cause immediate damage with total corneal opacification with conjunctival ischemia, and with corneal stromal edema within an hour, followed by necrosis of anterior ocular structures. An 8% solution produced ischemia and corneal stromal edema persisting for 40-65 days, accompanied by corneal vascularization. Even a 2% solution caused mild persistent stromal edema and vascularization. (6, 11)	
Category 1(H)	Sulfuric acid	At aerosol concentrations of 1.1 to 2.1 mg/cu m, 40% of human subjects noticed irritation of the eyes. At 2.4 to 6.0 mg/cu m, all subjects experienced eye irritation. Contact of concentrated sulfuric acid with the eye may cause total loss of vision in addition to corneal necrosis, opacification, scarring, ulceration and vascularization. (1, 44, 51, 52)	Animals in the vicinity of potato fields sprayed with sulfuric acid during spraying, or gaining access to such fields soon after spraying, may develop eye burns from the spray. (63)	
Category 1(H)	Zinc chloride	An unstated concentration of zinc chloride solution splashed in 1 eye of a workman at first only caused redness and discomfort, but within 6 days grayish corneal opacities had developed, with irregularity of the overlying epithelium. A patient who had an eye burned with one drop of 50% zinc chloride solution there was immediate severe pain, erosion of the corneal epithelium, corneal vascularization, severe iritis and iridial hemorrhage (11, 27, 54)	10% zinc chloride was classified as a mild or non-irritant when test in the rabbit eye. A 50% solution of zinc chloride applied repeatedly during 1 day to 1 eye of an albino rabbit caused immediate corneal opacity. 6 days after exposure, the eye had become very hard, with extensive hemorrhage in the anterior segment, accompanied by infiltration with inflammatory cells, loss of corneal endothelium and clouding of the anterior portion of the lens. (11, 61)	
Category 2A	Methyl acetate	Cases of slight poisoning under industrial conditions were manifested by eye burns and laceration. One case of blindness has been reported. (1, 13, 18)		

GHS Classification	Substance	CASRN	In Vivo Data Source	Substance Source	Commercial Availability	Chemical Class	Product Class	Conc. Tested	Amount Tested ^a	Purity	MW	pH	Dermal Corrosivity	# of Animals Tested	Water Solubility	Log Kow	Color
Category 2A	Acetone	67-64-1	ECETOC	Fisher Scientific International, Inc.	Sigma-Aldrich Corp.	Ketone	Chemical Intermediate, Cleaning Agent, Industrial Chemical, Pharmaceutical Intermediate, Preservative, Solvent	100%	0.1 mL	99%	58.1	5.3	noncorrosive	4	soluble	-0.24	?
Category 2A	Benzotrichloride	98-07-7	TSCA	Velsicol Chemical Corp.	Sigma-Aldrich Corp.	Hydrocarbon (cyclic)	Chemical Intermediate	100%	0.1 mL	n.a.	195.5	?	?	6	?	?	?
Category 2A	iso-Butanol	78-83-1	ECETOC	n.a.	Sigma-Aldrich Corp.	Alcohol	Chemical Intermediate, Food Additive, Pesticide, Pharmaceutical Intermediate, Solvent	100%	0.1 mL	99.9%	74.1	7.0	noncorrosive	4	soluble (95 g/L)	0.76	?
Category 2A	n-Butanol	71-36-3	ECETOC	Fisher Scientific International, Inc.	Sigma-Aldrich Corp.	Alcohol	Chemical Intermediate, Cosmetic Ingredient, Food Additive, Industrial Chemical, Pesticide Intermediate, Pharmaceutical Intermediate, Solvent, Veterinary Chemical	100%	0.1 mL	99.8%	74.1	n.a.	noncorrosive	4	insoluble	0.88	colorless
Category 2A	gamma-Butyrolactone	96-48-0	ECETOC	Shell Oil Co. of California	Sigma-Aldrich Corp.	Heterocyclic Compound, Lactone	Solvent	100%	0.1 mL	>99%	86.1	4.5	noncorrosive	6	miscible	-0.57	colorless
Category 2A	4-Carboxybenzaldehyde	619-66-9	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Aldehyde, Acid (organic) [carboxylic acid]	Industrial Chemical	100%	0.1 mL	>95%	150.1	3.1	noncorrosive	3	Very soluble	n.a.	?
Category 2A	Cetylpyridinium bromide	140-72-7	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Onium Compound, Heterocyclic Compound	Anti-Infective; Laboratory Chemical; Surfactant (cationic)	1%	0.1 mL	99%	384.4	6.4	noncorrosive	6	soluble (5 g/L)	1.83 (100%)	faintly beige
Category 2A	Deoxycholic acid sodium salt	302-95-4	LNS	n.a.	Sigma-Aldrich Corp.	Alcohol, Acid (organic) [carboxylic acid], Polycyclic Compound, Salt (organic)	Anti-Infective, Laboratory Chemical, Salt (organic)	10%	0.1 mL	n.a.	414.6	?	?	3	?	?	?
Category 2A	Dibenzyl phosphate	1623-08-1	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Ester, Organophosphorus Compound	Pesticide	100%	100 mg	99%	278.2	2.4	noncorrosive	3	n.a.	n.a.	?
Category 2A	2,6-Dichlorobenzoyl chloride	4659-45-4	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Acyl Halide	Anti-Fungal, Anti-Infective	100%	0.1 mL	99%	209.5	2.5	R34	6	insoluble	2.57	slight yellow
Category 2A	2-Ethyl-1-hexanol	104-76-7	ECETOC	Fisher Scientific International, Inc.	Sigma-Aldrich Corp.	Alcohol	Solvent	100%	0.1 mL	99%	130.2	4.8	noncorrosive	4	slightly soluble	2.82	?
Category 2A	n-Hexanol	111-27-3	ECETOC	Kodak Co.	Sigma-Aldrich Corp.	Alcohol	Solvent	100%	0.1 mL	98%	102.2	5.5	noncorrosive	4	soluble (5.8 g/L)	2.03	?
Category 2A	Methyl ethyl ketone	78-93-3	ECETOC	Fisher Scientific International, Inc.	Sigma-Aldrich Corp.	Ketone	Solvent	100%	0.1 mL	99%	72.1	5.5	noncorrosive	4	soluble (353 g/L)	0.29	colorless
Category 2A	Methyl cyanoacetate	105-34-0	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Ester, Nitrile	Chemical Intermediate	100%	0.1 mL	99%	99.1	5.7	noncorrosive	3	soluble (54 g/L)	n.a.	light yellow
Category 2A	n-Octanol	111-87-5	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Alcohol	Solvent	100%	0.1 mL	>99%	130.2	6.1	noncorrosive	3	insoluble (540 mg/L)	3.00	?
Category 2A	Triton X-100	9002-93-1	ECETOC	n.a.	Sigma-Aldrich Corp.	Ether	Surfactant (nonionic)	5%	0.1 mL	98%	250.4	n.a.	noncorrosive	6	soluble	n.a.	colorless
Category 2B	Methyl acetate	79-20-9	ZEBET	n.a.	Sigma-Aldrich Corp.	Ester	Chemical Intermediate, Food Additive, Herbicide, Laboratory Chemical, Solvent	n.a.	0.1 mL	n.a.	74.1	7.0	?	3	243 g/L	0.18	colorless
Category 2B	Ethyl-2-methyl acetoacetate	609-14-3	ECETOC	Fluka, Inc.	Sigma-Aldrich Corp.	Ester, Ketone	Chemical Intermediate	100%	0.1 mL	97%	144.2	7.5	noncorrosive	3	Slightly soluble	n.a.	?
Category 2B	Acetoacetic acid glycol ester	5459-04-1	ZEBET	n.a.	Hoechst Celanese Corp. (Bulk)	Ester, Ketone	Chemical Intermediate, Pesticide	n.a.	0.1 mL or 100 mg	n.a.	230.2	?	?	3	?	?	?
Category 2B	Ammonium nitrate	6484-52-2	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Onium Compound, Nitrate, Salt (organic)	Industrial Chemical	100%	100 mg	#####	80.0	4.8	noncorrosive	3	soluble (1920 g/L)	n.a.	white, hot concentrate
Category 2B	n-Butanal	123-72-8	ZEBET	n.a.	Sigma-Aldrich Corp.	Aldehyde	Chemical Intermediate, Food Additive	n.a.	0.1 mL or 100 mg	n.a.	72.1	?	?	3	?	?	?
Category 2B	Butyl Dipropyl Solvent	29911-27-1	TSCA	Union Carbide Corp.	Sigma-Aldrich Corp.	Alcohol, Ether	Solvent	100%	0.1 mL	99%	176.3	?	?	6	?	?	?
Category 2B	Camphen	79-92-5	ZEBET	n.a.	Sigma-Aldrich Corp.	Hydrocarbon (cyclic)	Chemical Intermediate, Cosmetic Ingredient, Food Additive, Pesticide Intermediate	n.a.	0.1 mL or 100 mg	n.a.	136.2	?	?	3	?	?	colorless
Category 2B	3-Chloropropionitrile	542-76-7	ECETOC	Fluka, Inc.	Sigma-Aldrich Corp.	Nitrile	Chemical Intermediate, Pharmaceutical Intermediate	100%	0.1 mL	99.9%	89.5	n.a.	noncorrosive	3	soluble (45 g/100 mL)	0.18	?
Category 2B	Cyclopentanol	96-41-3	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Alcohol	Pharmaceutical Intermediate	100%	0.1 mL	99%	86.1	n.a.	noncorrosive	3	slightly soluble	0.71	colorless
Category 2B	m-Dinitrobenzene	99-65-0	ZEBET	n.a.	Sigma-Aldrich Corp.	Nitro Compound	Chemical Intermediate	n.a.	0.1 mL or 100 mg	n.a.	168.1	?	?	3	?	?	?

GHS Classification	Substance	Physical Form Tested	MMAS score	Corneal score	Irital score	Conjunctival score	NICEATM Category 1 SubClass.2	Tested in BCOP	Tested in HET-CAM	Tested in ICE	Tested in IRE	EPA Classification	EU Classification	FHSA Classification
Category 2A	Acetone	liquid	65.8	-	-	-	-	X	X	X	X	Category II	R36	SCNM
Category 2A	Benzotrichloride	liquid	11.7	-	-	-	-	-	-	-	-	Category II	nonirritant	irritant
Category 2A	iso-Butanol	liquid	60.3	-	-	-	-	-	X	X	X	Category I	R41	SCNM
Category 2A	n-Butanol	liquid	60.8	-	-	-	-	-	X	X	X	Category II	R36	SCNM
Category 2A	gamma-Butyrolactone	liquid	43.0	-	-	-	-	X	X	X	X	Category II	R36	irritant
Category 2A	4-Carboxybenzaldehyde	liquid	50.3	-	-	-	-	X	X	X	-	Category II	R36	SCNM
Category 2A	Cetylpyridinium bromide	liquid	36.0	-	-	-	-	-	X	-	X	SCNM	R41	SCNM
Category 2A	Deoxycholic acid sodium salt	liquid	38.0	-	-	-	-	X	-	-	-	Category II	R36	SCNM
Category 2A	Dibenzyl phosphate	solid	30.0	-	-	-	-	X	-	X	-	Category II	R36	SCNM
Category 2A	2,6-Dichlorobenzoyl chloride	liquid	23.8	-	-	-	-	X	X	X	-	Category II	R36	irritant
Category 2A	2-Ethyl-1-hexanol	liquid	51.3	-	-	-	-	X	X	X	-	Category II	R36	SCNM
Category 2A	n-Hexanol	liquid	64.8	-	-	-	-	X	X	X	X	Category II	R36	SCNM
Category 2A	Methyl ethyl ketone	liquid	50.0	-	-	-	-	X	X	X	X	Category III	R36	SCNM
Category 2A	Methyl cyanoacetate	liquid	27.7	-	-	-	-	X	X	X	-	Category II	R36	SCNM
Category 2A	n-Octanol	liquid	41.0	-	-	-	-	X	X	X	X	Category II	R36	SCNM
Category 2A	Triton X-100	liquid	33.8	-	-	-	-	-	X	X	X	Category I	R41	SCNM
Category 2B	Methyl acetate	liquid	16.3	-	-	-	-	-	-	-	-	Category III	R36	Insufficient Animal Data
Category 2B	Ethyl-2-methyl acetoacetate	liquid	18.0	-	-	-	-	X	X	X	X	Category III	nonirritant	SCNM
Category 2B	Acetoacetic acid glycol ester	?	13.7	-	-	-	-	-	-	-	-	Category III	R36	SCNM
Category 2B	Ammonium nitrate	solid	18.3	-	-	-	-	X	X	X	X	Category III	R36	SCNM
Category 2B	n-Butanal	liquid	12.7	-	-	-	-	-	X	-	-	Category III	nonirritant	SCNM
Category 2B	Butyl Dipropasol Solvent	liquid	24.7	-	-	-	-	-	-	-	-	Category III	nonirritant	irritant
Category 2B	Camphen	solid	15.0	-	-	-	-	-	X	-	-	Category III	R36	SCNM
Category 2B	3-Chloropropionitrile	liquid	13.7	-	-	-	-	-	-	-	-	Category III	nonirritant	SCNM
Category 2B	Cyclopentanol	liquid	21.7	-	-	-	-	-	-	X	-	Category II	R36	SCNM
Category 2B	m-Dinitrobenzene	solid	15.7	-	-	-	-	-	-	-	-	Category III	R36	SCNM

GHS Classification	Substance	Human Exposure Summary	Animal Exposure Summary for Category 1(H) Substances	Notes
Category 2A	Acetone	Acute exposures of humans to atmospheric concentrations have been reported to produce eye irritation. Exposure of 15 minutes to aerosol concentrations of 1660 ppm also reportedly causes eye irritation. Direct contact with the eyes may produce irritation and corneal injury. (14, 16, 30, 32)		
Category 2A	Benzotrichloride	Human data not located		
Category 2A	iso-Butanol	Irritation of the skin, eyes, and throat have been reported from exposure to vapor or liquid. Irritation of the eyes and throat, formation of vacuoles in the superficial layers of the cornea, were reported among workers subjected to an undetermined, but apparently high concn of isobutyl alcohol & butyl acetate. (9, 20)+AH12		Discordant GHS classification
Category 2A	n-Butanol	Is reported to cause irritation of the eyes from exposure to either vapor or liquid. Circumstantial evidence points to butyl alcohol vapor as cause of a special vacuolar keratopathy in some patients; the most severely affected it has been associated with pain & tearing, characteristically most marked on first opening eyes in morning. It can cause transient mild edema of conjunctiva of the eye. Vapor: Irritating to eyes. Considered a strong irritant of the eyes. (9, 11, 13, 27)		Used results when tested at lower concentration
Category 2A	gamma-Butyrolactone	Human data not located		
Category 2A	4-Carboxybenzaldehyde	Human data not located		
Category 2A	Cetylpyridinium bromide	Human data not located		
Category 2A	Deoxycholic acid sodium salt	Human data not located		
Category 2A	Dibenzyl phosphate	Human data not located		
Category 2A	2,6-Dichlorobenzoyl chloride	Human data not located		
Category 2A	2-Ethyl-1-hexanol	Irritation of eyes from vapor or liquid (8, 9)		
Category 2A	n-Hexanol	Reported to cause eye burns (27)		
Category 2A	Methyl ethyl ketone	High atmospheric concentrations are irritating to the eyes. May produce painful irritation and corneal injury if splashed in the eyes. Workers exposed to 33,000 and 100,000 ppm in air reported intolerable irritation of the eyes. Implicated as the cause of retrobulbar neuritis in one patient. A workman splashed his eye accidentally with methyl ethyl ketone, but the next day had only slight conjunctival hyperemia and no residual corneal injury. (2, 5, 11, 20)		
Category 2A	Methyl cyanoacetate	Human data not located		
Category 2A	n-Octanol	Has caused injury of the corneal epithelium, with recovery in 48 hours (11)		
Category 2A	Triton X-100	Human data not located		
Category 2B	Methyl acetate	Cases of slight poisoning under industrial conditions were manifested by eye burns and lacrimation. One case of blindness has been reported. (1, 13, 18)		Conc. tested unknown
Category 2B	Ethyl-2-methyl acetoacetate	Human data not located		
Category 2B	Acetoacetic acid glycol ester	?	?	
Category 2B	Ammonium nitrate	Human data not located		
Category 2B	n-Butanal	?	?	Conc. tested unknown
Category 2B	Butyl Dipropasol Solvent	Human data not located		
Category 2B	Camphen	?	?	
Category 2B	3-Chloropropionitrile	Human data not located		
Category 2B	Cyclopentanol	Human data not located		
Category 2B	m-Dinitrobenzene	?	?	

GHS Classification	Substance	CASRN	In Vivo Data Source	Substance Source	Commercial Availability	Chemical Class	Product Class	Conc. Tested	Amount Tested ^a	Purity	MW	pH	Dermal Corrosivity	# of Animals Tested	Water Solubility	Log Kow	Color
Category 2B	3,3-Dithiodipropionic acid	1119-62-6	ECETOC	Fluka, Inc.	Sigma-Aldrich Corp.	Acid (organic) [carboxylic acid], Organosilicon Compound	Chemical Intermediate, Laboratory Chemical	100%	100 mg	99%	210.3	pKa 3.94	R34	3	Very soluble	1.38	?
Category 2B	Hexyl cinnamic aldehyde	101-86-0	TSCA	Confidential	International Flavors and Fragrances, Inc. (Bulk)	Aldehyde	Cosmetic Ingredient, Food Additive, Perfume	12.5% in Alcohol	0.1 mL	n.a.	216.3	?	?	3	?	?	?
Category 2B	HZD Shampoo No. 5	n.a.	CTFA	Battelle Columbus Lab.	yes	Formulation	Shampoos, Hair	100%	0.1 mL	n.a.	n.a.	n.a.	n.a.	3	n.a.	n.a.	n.a.
Category 2B	Isopropyl acetoacetate	542-08-5	ZEBET	n.a.	Sigma-Aldrich Corp.	Ester, Ketone	Chemical Intermediate	n.a.	0.1 mL or 100 mg	n.a.	144.2	?	?	3	?	?	?
Category 2B	N-Laurylsarcosine sodium salt	137-16-6	LNS	n.a.	Sigma-Aldrich Corp.	Amide, Amine, Salt (organic)	Cleaning Agent, Detergent, Laboratory Chemical, Surfactant (anionic)	10%	0.1 mL	n.a.	293.4	?	?	3	?	?	?
Category 2B	Maneb (solid)	12427-38-2	ECETOC	US EPA	Sigma-Aldrich Corp.	Amine, Salt (organic), Urea	Pesticide	100%	100 mg	90% (approx)	265.3	8.4	noncorrosive	6	Moderately soluble	n.a.	?
Category 2B	2-Methyl-1-pentanol	105-30-6	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Alcohol	Solvent	100%	0.1 mL	99%	102.2	n.a.	noncorrosive	3	soluble (6 g/L)	1.75	?
Category 2B	p-Nitrobenzoic acid	62-23-7	ZEBET	n.a.	Sigma-Aldrich Corp.	Acid (organic) [carboxylic acid], Nitro Compound	Chemical Intermediate, Pharmaceutical Intermediate	n.a.	0.1 mL or 100 mg	n.a.	167.1	?	?	3	?	?	?
Category 2B	Propasol Solvent P	1569-01-3	TSCA	Union Carbide Corp.	Sigma-Aldrich Corp.	Alcohol	Solvent	100%	0.1 mL	n.a.	118.2	?	?	6	?	?	?
Category 2B	6-Methyl purine	2004-03-7	TSCA	Monsanto Co.	Sigma-Aldrich Corp.	Heterocyclic Compound	Laboratory Chemical, Pharmaceutical Intermediate	100%	0.1 mL	n.a.	134.1	-	-	6	?	?	?
Category 2B	2,6-Dichloro-5-fluoro-beta-oxo-3-pyridinepropanoate	96568-04-6	GSK	n.a.	Sigma-Aldrich Corp.	Ester, Heterocyclic Compound, Ketone	Industrial Chemical, Pharmaceutical Intermediate	100%	0.1 mL or 100 mg	n.a.	280.1	?	?	3	?	?	white
Category 2B	Sodium monochloroacetate	3926-62-3	ZEBET	n.a.	Sigma-Aldrich Corp.	Acid (organic) [carboxylic acid], Salt (organic)	Chemical Intermediate, Herbicide, Pharmaceutical Intermediate	n.a.	0.1 mL or 100 mg	n.a.	116.5	?	?	3	?	?	?
Category 2B	Triton X-100	9002-93-1	ECETOC	n.a.	Sigma-Aldrich Corp.	Ether	Surfactant (nonionic)	5%	0.1 mL	98%	250.4	n.a.	noncorrosive	6	soluble	n.a.	colorless
nonirritant	Ethyl trimethyl acetate	3938-95-2	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Ester	Industrial Chemical	100%	0.1 mL	99%	130.2	?	?	6	?	?	?
nonirritant	iso-Octyl acrylate	29590-42-9	ECETOC	Elf Atochem, Inc.	Sigma-Aldrich Corp.	Ester	Building Material	100%	0.1 mL	>99%	184.3	n.a.	noncorrosive	3	n.a.	n.a.	?
nonirritant	Iso-myristyl alcohol	5333-48-2	ECETOC	Elf Atochem, Inc.	Elf Atochem, Inc. (Bulk)	Alcohol	Industrial Chemical, Solvent	100%	0.1 mL	92.6%	n.a.	?	?	3	?	?	?
nonirritant	tetra-Aminopyrimidine sulfate	5392-28-9	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Amine, Heterocyclic Compound, Salt (organic)	Chemical Intermediate	100%	100 mg	97%	238.2	n.a.	noncorrosive	3	slightly soluble	n.a.	?
nonirritant	n-Amyl bromide	110-53-2	ECETOC	Elf Atochem, Inc.	Sigma-Aldrich Corp.	Hydrocarbon (halogenated)	Chemical Intermediate, Pharmaceutical Intermediate, Solvent	100%	0.1 mL	>98.5%	151.0	?	?	3	?	?	?
nonirritant	1,3-Di-iso-propyl benzene	99-62-7	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Hydrocarbon (cyclic)	Chemical Intermediate, Solvent	100%	0.1 mL	96%	162.3	?	?	6	soluble with Alcohol, Ether, acetone	?	?
nonirritant	4-Bromophenetole	589-10-6	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Ether	Chemical Intermediate	100%	0.1 mL	99%	201.1	?	?	3	?	?	?
nonirritant	Bromo-2-butane	78-76-2	ECETOC	Fluka, Inc.	Sigma-Aldrich Corp.	Hydrocarbon (halogenated)	Chemical Intermediate	100%	0.1 mL	>99%	137.0	?	?	3	?	?	?
nonirritant	n-Butyl acetate	123-86-4	ECETOC	Fisher Scientific International, Inc.	Sigma-Aldrich Corp.	Ester	Chemical Intermediate, Food Additive, Industrial Chemical, Pesticide, Solvent	100%	0.1 mL	99%	116.2	?	?	4	soluble in acetone, Ether, PPG	1.82	?
nonirritant	Cellosolve acetate	111-15-9	ECETOC	Fisher Scientific International, Inc.	Sigma-Aldrich Corp.	Ester, Ether	Chemical Intermediate, Pesticide, Pharmaceutical Intermediate, Preservative, Solvent	100%	0.1 mL	99%	305.8	?	?	4	230 g/L	?	?
nonirritant	Cetylpyridinium bromide	140-72-7	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Onium Compound, Heterocyclic Compound	Anti-Infective; Laboratory Chemical; Surfactant (cationic)	0.10%	0.1 mL	99%	384.4	4.8	noncorrosive	4	soluble (5 g/L)	1.83 (100%)	faintly beige
nonirritant	Chlorendic anhydride	115-27-5	TSCA	Velsicol Chemical Corp.	Sigma-Aldrich Corp.	Anhydride	Chemical Intermediate, Flame Retardant	n.a.	100 mg	98.8%	370.8	?	?	6	?	?	?
nonirritant	1-Bromo-4-chlorobutane	6940-78-9	ECETOC	Fluka, Inc.	Sigma-Aldrich Corp.	Hydrocarbon (halogenated)	Industrial Chemical	100%	0.1 mL	98%	171.5	?	?	3	soluble in ethanol, ethyl ether	?	colorless to yellow
nonirritant	Chlorpyrifos	2921-88-2	TSCA	Dow Chemical Co.	Sigma-Aldrich Corp.	Organophosphorus Compound	Pesticide	100%	0.1 mL	#####	350.6	?	?	6	?	?	white
nonirritant	Methyl cyclopentane	96-37-7	ECETOC	Fluka, Inc.	Sigma-Aldrich Corp.	Hydrocarbon (cyclic)	Solvent	100%	0.1 mL	>99%	84.2	?	?	6	?	?	colorless
nonirritant	1,9-Decadiene	1647-16-1	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Hydrocarbon (acyclic)	Chemical Intermediate	100%	0.1 mL	98%	138.3	?	?	6	?	?	?
nonirritant	1,4-Dibromobutane	110-52-1	ECETOC	Fluka, Inc.	Sigma-Aldrich Corp.	Hydrocarbon (halogenated)	Chemical Intermediate, Industrial Chemical, Laboratory Chemical	100%	0.1 mL	99.9%	215.9	?	?	3	insoluble	?	?
nonirritant	1,6-Dibromohexane	629-03-8	ECETOC	Fluka, Inc.	Sigma-Aldrich Corp.	Hydrocarbon (halogenated)	Chemical Intermediate, Pharmaceutical Intermediate	100%	0.1 mL	98.4%	244.0	?	?	3	insoluble	?	colorless to yellow
nonirritant	1,5-Dibromopentane	111-24-0	ECETOC	Fluka, Inc.	Sigma-Aldrich Corp.	Hydrocarbon (halogenated)	Pharmaceutical Intermediate	100%	0.1 mL	99.5%	230.0	?	?	3	insoluble	?	?

GHS Classification	Substance	Physical Form Tested	MMAS score	Corneal score	Irital score	Conjunctival score	NICEATM Category 1 SubClass.2	Tested in BCOP	Tested in HET-CAM	Tested in ICE	Tested in IRE	EPA Classification	EU Classification	FHSA Classification
Category 2B	3,3-Dithiodipropionic acid	solid	31.7	-	-	-	-	-	-	-	-	Category II	nonirritant	SCNM
Category 2B	Hexyl cinnamic aldehyde	liquid	21.3	-	-	-	-	-	-	-	-	Category III	nonirritant	SCNM
Category 2B	HZD Shampoo No. 5	liquid	33.7	-	-	-	-	-	X	-	-	Category III	nonirritant	SCNM
Category 2B	Isopropyl acetoacetate	?	12.0	-	-	-	-	-	-	-	-	Category III	nonirritant	SCNM
Category 2B	N-Laurylsarcosine sodium salt	liquid	31.0	-	-	-	-	X	-	-	-	Category III	nonirritant	SCNM
Category 2B	Maneb (solid)	solid	14.3	-	-	-	-	X	X	X	X	Category III	R36	irritant
Category 2B	2-Methyl-1-pentanol	liquid	13.0	-	-	-	-	-	-	-	-	Category III	nonirritant	SCNM
Category 2B	p-Nitrobenzoic acid	solid	19.3	-	-	-	-	-	-	-	-	Category III	nonirritant	SCNM
Category 2B	Propasol Solvent P	liquid	31.2	-	-	-	-	-	-	-	-	Category II	nonirritant	irritant
Category 2B	6-Methyl purine	liquid	48.7	-	-	-	-	-	-	-	-	Category IV	R36	irritant
Category 2B	2,6-Dichloro-5-fluoro-beta-oxo-3-pyridinepropanoate	solid	21.3	-	-	-	-	-	-	-	-	Category III	nonirritant	SCNM
Category 2B	Sodium monochloroacetate	solid	15.7	-	-	-	-	-	X	-	-	Category III	R36	SCNM
Category 2B	Triton X-100	liquid	33.8	-	-	-	-	-	X	X	X	Category I	R41	SCNM
nonirritant	Ethyl trimethyl acetate	liquid	3.8	-	-	-	-	-	X	X	-	Category III	nonirritant	nonirritant
nonirritant	iso-Octyl acrylate	liquid	5.3	-	-	-	-	-	-	-	-	Category IV	nonirritant	SCNM
nonirritant	Iso-myristyl alcohol	liquid	8.0	-	-	-	-	-	-	-	-	Category III	nonirritant	SCNM
nonirritant	tetra-Aminopyrimidine sulfate	solid	10.3	-	-	-	-	X	X	X	-	Category III	nonirritant	SCNM
nonirritant	n-Amyl bromide	liquid	4.0	-	-	-	-	-	-	-	-	Category IV	nonirritant	SCNM
nonirritant	1,3-Di-iso-propyl benzene	liquid	2.0	-	-	-	-	-	-	-	-	Category IV	nonirritant	nonirritant
nonirritant	4-Bromophenetole	liquid	1.3	-	-	-	-	-	-	-	-	Category IV	nonirritant	SCNM
nonirritant	Bromo-2-butane	liquid	0.0	-	-	-	-	-	-	-	-	Category IV	nonirritant	SCNM
nonirritant	n-Butyl acetate	liquid	7.5	-	-	-	-	X	X	X	X	Category III	nonirritant	SCNM
nonirritant	Cellosolve acetate	liquid	15.0	-	-	-	-	-	-	-	-	Category III	nonirritant	SCNM
nonirritant	Cetylpyridinium bromide	liquid	2.7	-	-	-	-	X	X	-	-	Category I	R41	irritant
nonirritant	Chlorendic anhydride	solid	21.8	-	-	-	-	-	-	-	-	Category II	R36	irritant
nonirritant	1-Bromo-4-chlorobutane	liquid	4.0	-	-	-	-	-	-	-	-	Category IV	nonirritant	SCNM
nonirritant	Chlorpyrifos	liquid	0.0	-	-	-	-	-	-	-	-	Category IV	nonirritant	nonirritant
nonirritant	Methyl cyclopentane	liquid	3.7	-	-	-	-	X	X	X	-	Category III	nonirritant	nonirritant
nonirritant	1,9-Decadiene	liquid	5.7	-	-	-	-	-	-	-	-	Category IV	nonirritant	nonirritant
nonirritant	1,4-Dibromobutane	liquid	6.0	-	-	-	-	-	-	-	-	Category III	nonirritant	SCNM
nonirritant	1,6-Dibromohexane	liquid	6.7	-	-	-	-	-	-	-	-	Category IV	nonirritant	SCNM
nonirritant	1,5-Dibromopentane	liquid	4.7	-	-	-	-	-	-	-	-	Category III	nonirritant	SCNM

GHS Classification	Substance	Human Exposure Summary	Animal Exposure Summary for Category 1(H) Substances	Notes
Category 2B	3,3-Dithiodipropionic acid	Human data not located		
Category 2B	Hexyl cinnamic aldehyde	Human data not located		
Category 2B	HZD Shampoo No. 5	?	?	Formulations excluded.
Category 2B	Isopropyl acetoacetate	?	?	
Category 2B	N-Laurylsarcosine sodium salt	Human data not located		
Category 2B	Maneb (solid)	Generally regarded as harmless, with no irritation, except for mild conjunctivitis (9)		
Category 2B	2-Methyl-1-pentanol	Human data not located		
Category 2B	p-Nitrobenzoic acid	?	?	
Category 2B	Propasol Solvent P	Human data not located		
Category 2B	6-Methyl purine	Human data not located		
Category 2B	2,6-Dichloro-5-fluoro-beta-oxo-3-pyridinepropanoate	Human data not located		
Category 2B	Sodium monochloroacetate	?	?	
Category 2B	Triton X-100	Human data not located		
nonirritant	Ethyl trimethyl acetate	?	?	
nonirritant	iso-Octyl acrylate	Human data not located		
nonirritant	Iso-myristyl alcohol	?	?	
nonirritant	tetra-Aminopyrimidine sulfate	Human data not located		
nonirritant	n-Amyl bromide	?	?	
nonirritant	1,3-Di-iso-propyl benzene	?	?	
nonirritant	4-Bromophenetole	?	?	
nonirritant	Bromo-2-butane	?	?	
nonirritant	n-Butyl acetate	?	?	
nonirritant	Cellosolve acetate	Human data not located		
nonirritant	Cetylpyridinium bromide	?	?	
nonirritant	Chlorendic anhydride	?	?	
nonirritant	1-Bromo-4-chlorobutane	?	?	
nonirritant	Chlorpyrifos	?	?	
nonirritant	Methyl cyclopentane	?	?	
nonirritant	1,9-Decadiene	?	?	
nonirritant	1,4-Dibromobutane	?	?	
nonirritant	1,6-Dibromohexane	?	?	
nonirritant	1,5-Dibromopentane	?	?	

GHS Classification	Substance	CASRN	In Vivo Data Source	Substance Source	Commercial Availability	Chemical Class	Product Class	Conc. Tested	Amount Tested ^a	Purity	MW	pH	Dermal Corrosivity	# of Animals Tested	Water Solubility	Log Kow	Color
nonirritant	1,3-Dibromopropane	109-64-8	ECETOC	Fluka, Inc.	Sigma-Aldrich Corp.	Hydrocarbon (halogenated)	Chemical Intermediate, Pesticide Intermediate, Pharmaceutical Intermediate	100%	0.1 mL	98.4%	201.9	?	?	3	1.7 g/L	?	?
nonirritant	Dichlorotoluenes	mixture of isomers	ECETOC	Elf Atochem, Inc.	Elf Atochem, Inc. (Bulk)	Hydrocarbon (halogenated)	Industrial Chemical	100%	0.1 mL	99-99.8%	n.a.	?	?	3	?	?	?
nonirritant	2,4-Difluoronitrobenzene	446-35-5	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Hydrocarbon (halogenated)	Pesticide, Pharmaceutical Intermediate	100%	0.1 mL	99%	159.1	n.a.	noncorrosive	6	n.a.	n.a.	n.a.
nonirritant	1-(4-Phenyl-phenoxy)-1-(1,2,4-triazole-1)-3,3-dimethylbutane	55179-31-2	TSCA	Mobay Corp.	Shanghai Orchem Co., Ltd.	Heterocyclic Compound	Anti-Fungal, Pesticide	100%	0.1 mL	96.5%	337.4	?	?	3	?	?	?
nonirritant	n,n-Dimethylguanidine sulfate	598-65-2	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Amidine, Salt (organic)	Laboratory Chemical	100%	100 mg	>95%	272.3	n.a.	noncorrosive	3	n.a.	n.a.	n.a.
nonirritant	3,3-Dimethylpentane	562-49-2	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Hydrocarbon (acyclic)	Chemical Intermediate	100%	0.1 mL	99%	100.2	?	?	3	insoluble	?	?
nonirritant	2,3-Dimethyl 2,3-dinitrobutane	3964-18-4	TSCA	Dow Chemical Co.	Dow Chemical Co. (Bulk)	Nitro Compound	Industrial Chemical	100%	100 mg	>95%	176.2	?	?	6	?	?	?
nonirritant	Di-n-propyl disulfide	629-19-6	ECETOC	Fluka, Inc.	Sigma-Aldrich Corp.	Sulfur Compound (organic)	Food Additive, Industrial Agent	100%	0.1 mL	99.2%	150.3	?	?	3	insoluble	?	colorless
nonirritant	n-Dodecane	112-40-3	ECETOC	Fluka, Inc.	Sigma-Aldrich Corp.	Hydrocarbon (acyclic)	Chemical Intermediate, Solvent	100%	0.1 mL	>99.5%	170.3	?	?	6	?	?	?
nonirritant	2-(n-Dodecylthio)ethanol	1462-55-1	ECETOC	Elf Atochem, Inc.	Sigma-Aldrich Corp.	Alcohol, Ether, Sulfur Compound (organic)	Chemical Intermediate	100%	100 mg	>99%	206.3	?	?	3	?	?	white
nonirritant	2-Ethoxyethyl methacrylate	2370-63-0	ECETOC	Elf Atochem, Inc.	Sigma-Aldrich Corp.	Ester, Ether	Dental Adhesive	100%	0.1 mL	99.8%	158.2	n.a.	noncorrosive	3	n.a.	n.a.	?
nonirritant	Ethyl acetate	141-78-6	ECETOC	Fisher Scientific International, Inc.	Sigma-Aldrich Corp.	Ester	Cleaning Agent, Food Additive, Solvent	100%	0.1 mL	99%	88.1	?	?	4	80 g/L	?	colorless
nonirritant	Ethyl thioglycolate	623-51-8	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Alcohol, Ester, Sulfur Compound (organic)	Chemical Intermediate, Cosmetic Ingredient, Food Additive, Industrial Chemical	100%	0.1 mL	99.1%	120.2	?	?	3	?	?	?
nonirritant	Ethylene glycol diethyl ether	629-14-1	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Ether	Chemical Intermediate, Solvent	100%	0.1 mL	98%	118.2	?	?	3	?	?	colorless
nonirritant	2-Ethylhexylthioglycolate	7659-86-12	ECETOC	Elf Atochem, Inc.	Elf Atochem, Inc. (Bulk)	Alcohol, Ester, Sulfur Compound (organic)	Chemical Intermediate, Cosmetic Ingredient	100%	0.1 mL	99.4%	204.3	?	?	3	?	?	?
nonirritant	Glycerol	56-81-5	ECETOC	Mallinckrodt, Inc.	Sigma-Aldrich Corp.	Alcohol	Chemical Intermediate, Cosmetic Ingredient, Food Additive, Pharmaceutical, Solvent	100%	0.1 mL	>99.5%	92.1	6.0-7.0 (10% aq.)	?	6	>500 g/L	?	?
nonirritant	Glycidyl methacrylate	106-91-2	ECETOC	Elf Atochem, Inc.	Sigma-Aldrich Corp.	Ether	Chemical Intermediate, Dental Adhesive, Industrial Chemical	100%	0.1 mL	>99%	142.2	?	?	3	?	?	?
nonirritant	1,5-Hexadiene	592-42-7	ECETOC	Fluka, Inc.	Sigma-Aldrich Corp.	Hydrocarbon (acyclic)	Chemical Intermediate, Industrial Chemical	100%	0.1 mL	97%	82.2	?	?	6	?	?	?
nonirritant	Perfluoro-n-hexane	355-42-0	TSCA	3M Corp.	Fisher Scientific International, Inc.	Hydrocarbon (halogenated)	Industrial Chemical	100%	0.1 mL	>90%	338.0	?	?	3	?	?	?
nonirritant	Perfluoro-n-hexane	355-42-0	TSCA	3M Corp.	Fisher Scientific International, Inc.	Hydrocarbon (halogenated)	Industrial Chemical	100%	0.1 mL	90%	338.0	?	?	3	?	?	?
nonirritant	n-Hexyl bromide	111-25-1	ECETOC	Fluka, Inc.	Sigma-Aldrich Corp.	Hydrocarbon (halogenated)	Industrial Chemical, Pharmaceutical Intermediate	100%	0.1 mL	>98.5%	165.1	?	?	3	?	?	?
nonirritant	iso-Propyl bromide	75-26-3	ECETOC	Fluka, Inc.	Sigma-Aldrich Corp.	Hydrocarbon (halogenated)	Chemical Intermediate, Pharmaceutical Intermediate	100%	0.1 mL	>99%	123.0	?	?	3	3 g/L	1.9	?
nonirritant	Di-iso-butyl ketone	108-83-8	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Ketone	Pharmaceutical Intermediate, Solvent	100%	0.1 mL	99%	142.2	n.a.	noncorrosive	3	0.05 g/100 mL	n.a.	?
nonirritant	Methyl iso-butyl ketone	108-10-1	ECETOC	Fisher Scientific International, Inc.	Sigma-Aldrich Corp.	Ketone	Food Additive, Solvent	100%	0.1 mL	98%	100.2	?	?	4	20 mg/mL	1.31	?
nonirritant	Allyl methacrylate	96-05-9	ECETOC	Elf Atochem, Inc.	Sigma-Aldrich Corp.	Ester	Chemical Intermediate	100%	0.1 mL	99.6%	126.2	?	?	6	4 g/L	?	?
nonirritant	Heptyl methacrylate	5459-37-0	ECETOC	Elf Atochem, Inc.	Elf Atochem, Inc. (Bulk)	Ester	Cosmetic Ingredient, Dental Adhesive, Perfume	100%	0.1 mL	>99%	164.3	?	?	3	?	?	?
nonirritant	Methyl trimethyl acetate	598-98-1	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Ester	Chemical Intermediate, Pharmaceutical Intermediate	100%	0.1 mL	99%	116.2	?	?	6	?	?	?
nonirritant	3-Methylhexane	589-34-4	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Hydrocarbon (acyclic)	Industrial Chemical	100%	0.1 mL	99%	100.2	?	?	6	insoluble	?	?
nonirritant	2-Methylpentane	107-83-5	ECETOC	Fluka, Inc.	Sigma-Aldrich Corp.	Hydrocarbon (acyclic)	Solvent	100%	0.1 mL	>99.5%	86.2	n.a.	noncorrosive	6	14 mg/L	3.74	?
nonirritant	1-Methylpropyl benzene	135-98-8	ECETOC	Fluka, Inc.	Sigma-Aldrich Corp.	Hydrocarbon (cyclic)	Solvent	100%	0.1 mL	>99.5%	134.2	?	?	6	0.015 g/L	?	?
nonirritant	p-Methylthio benzaldehyde	3446-89-7	ECETOC	Fluka, Inc.	Sigma-Aldrich Corp.	Aldehyde, Ether, Sulfur Compound (organic)	Chemical Intermediate	100%	0.1 mL	98.2%	152.2	?	?	3	?	?	?
nonirritant	Nonyl acrylate	2664-55-3	ECETOC	Elf Atochem, Inc.	Elf Atochem, Inc. (Bulk)	Ester	Industrial Chemical	100%	0.1 mL	99%	198.3	?	?	3	?	?	?
nonirritant	cis-Cyclo-octene	931-88-4	ECETOC	Fluka, Inc.	Sigma-Aldrich Corp.	Hydrocarbon (cyclic)	Chemical Intermediate, Industrial Chemical, Laboratory Chemical	100%	0.1 mL	95%	110.2	?	?	6	?	?	?
nonirritant	n-Octyl bromide	111-83-1	ECETOC	Fluka, Inc.	Sigma-Aldrich Corp.	Hydrocarbon (halogenated)	Chemical Intermediate, Industrial Chemical	100%	0.1 mL	>99%	193.1	?	?	3	?	?	?

GHS Classification	Substance	Physical Form Tested	MMAS score	Corneal score	Irital score	Conjunctival score	NICEATM Category 1 SubClass.2	Tested in BCOP	Tested in HET-CAM	Tested in ICE	Tested in IRE	EPA Classification	EU Classification	FHSA Classification
nonirritant	1,3-Dibromopropane	liquid	8.0	-	-	-	-	-	-	-	-	Category IV	nonirritant	SCNM
nonirritant	Dichlorotoluenes	liquid	0.0	-	-	-	-	-	-	-	-	Category IV	nonirritant	SCNM
nonirritant	2,4-Difluoronitrobenzene	solid	4.7	-	-	-	-	-	-	-	-	Category III	nonirritant	SCNM
nonirritant	1-(4-Phenyl-phenoxy)-1-(1,2,4-triazole-1)-3,3-dimethylbutane	liquid	5.7	-	-	-	-	-	-	-	-	Category III	nonirritant	nonirritant
nonirritant	n,n-Dimethylguanidine sulfate	solid	6.7	-	-	-	-	-	-	-	-	Category III	nonirritant	SCNM
nonirritant	3,3-Dimethylpentane	liquid	0.0	-	-	-	-	-	-	-	-	Category IV	nonirritant	SCNM
nonirritant	2,3-Dimethyl 2,3-dinitrobutane	solid	4.3	-	-	-	-	-	-	-	-	Category III	nonirritant	SCNM
nonirritant	Di-n-propyl disulfide	liquid	4.0	-	-	-	-	-	-	-	-	Category IV	nonirritant	SCNM
nonirritant	n-Dodecane	liquid	3.3	-	-	-	-	-	-	-	-	Category III	nonirritant	nonirritant
nonirritant	2-(n-Dodecylthio)ethanol	solid	0.0	-	-	-	-	-	-	-	-	Category IV	nonirritant	SCNM
nonirritant	2-Ethoxyethyl methacrylate	liquid	0.7	-	-	-	-	-	-	-	-	Category IV	nonirritant	SCNM
nonirritant	Ethyl acetate	liquid	15.0	-	-	-	-	X	X	X	X	Category III	nonirritant	SCNM
nonirritant	Ethyl thioglycolate	Liquid	24.7	-	-	-	-	-	-	-	-	Category III	nonirritant	SCNM
nonirritant	Ethyleneglycol diethyl ether	liquid	10.7	-	-	-	-	-	-	-	-	Category IV	nonirritant	SCNM
nonirritant	2-Ethylhexylthioglycolate	liquid	2.7	-	-	-	-	-	-	-	-	Category IV	nonirritant	SCNM
nonirritant	Glycerol	liquid	1.7	-	-	-	-	X	X	X	X	Category IV	nonirritant	nonirritant
nonirritant	Glycidyl methacrylate	Liquid	28.0	-	-	-	-	-	-	-	-	Category III	nonirritant	SCNM
nonirritant	1,5-Hexadiene	liquid	4.7	-	-	-	-	-	-	-	-	Category III	nonirritant	SCNM
nonirritant	Perfluoro-n-hexane	liquid	0.0	-	-	-	-	-	-	-	-	Category IV	nonirritant	Insufficient Animal Data
nonirritant	Perfluoro-n-hexane	liquid	0.0	-	-	-	-	-	-	-	-	Category IV	nonirritant	Insufficient Animal Data
nonirritant	n-Hexyl bromide	liquid	1.3	-	-	-	-	-	-	-	-	Category IV	nonirritant	SCNM
nonirritant	iso-Propyl bromide	liquid	9.7	-	-	-	-	-	-	-	-	Category IV	nonirritant	SCNM
nonirritant	Di-iso-butyl ketone	liquid	7.3	-	-	-	-	-	-	-	-	Category IV	nonirritant	SCNM
nonirritant	Methyl iso-butyl ketone	liquid	4.8	-	-	-	-	-	X	X	X	Category III	nonirritant	SCNM
nonirritant	Allyl methacrylate	liquid	5.8	-	-	-	-	-	-	-	-	Category III	nonirritant	SCNM
nonirritant	Heptyl methacrylate	liquid	1.3	-	-	-	-	-	-	-	-	Category IV	nonirritant	SCNM
nonirritant	Methyl trimethyl acetate	liquid	2.7	-	-	-	-	-	-	-	-	Category IV	nonirritant	nonirritant
nonirritant	3-Methylhexane	liquid	0.7	-	-	-	-	-	-	-	-	Category IV	nonirritant	nonirritant
nonirritant	2-Methylpentane	Liquid	2.3	-	-	-	-	-	-	-	-	Category IV	nonirritant	nonirritant
nonirritant	1-Methylpropyl benzene	liquid	3.7	-	-	-	-	-	-	-	-	Category IV	nonirritant	nonirritant
nonirritant	p-Methylthiobenzaldehyde	liquid	1.3	-	-	-	-	-	-	-	-	Category IV	nonirritant	SCNM
nonirritant	Nonyl acrylate	liquid	0.0	-	-	-	-	-	-	-	-	Category IV	nonirritant	SCNM
nonirritant	cis-Cyclo-octene	liquid	3.3	-	-	-	-	-	-	-	-	Category III	nonirritant	irritant
nonirritant	n-Octyl bromide	liquid	2.7	-	-	-	-	-	-	-	-	Category IV	nonirritant	SCNM

GHS Classification	Substance	Human Exposure Summary	Animal Exposure Summary for Category 1(H) Substances	Notes
nonirritant	1,3-Dibromopropane	?	?	
nonirritant	Dichlorotoluenes	?	?	
nonirritant	2,4-Difluoronitrobenzene	Human data not located		
nonirritant	1-(4-Phenyl-phenoxy)-1-(1,2,4-triazole-1)-3,3-dimethylbutane	?	?	
nonirritant	n,n-Dimethylguanidine sulfate	Human data not located		
nonirritant	3,3-Dimethylpentane	?	?	
nonirritant	2,3-Dimethyl 2,3-dinitrobutane	?	?	
nonirritant	Di-n-propyl disulfide	?	?	
nonirritant	n-Dodecane	?	?	
nonirritant	2-(n-Dodecylthio)ethanol	Human data not located		
nonirritant	2-Ethoxyethyl methacrylate	Human data not located		
nonirritant	Ethyl acetate	?	?	
nonirritant	Ethyl thioglycolate	?	?	
nonirritant	Ethyleneglycol diethyl ether	?	?	
nonirritant	2-Ethylhexylthioglycolate	?	?	
nonirritant	Glycerol	?	?	
nonirritant	Glycidyl methacrylate	?	?	
nonirritant	1,5-Hexadiene	?	?	
nonirritant	Perfluoro-n-hexane	?	?	
nonirritant	Perfluoro-n-hexane	?	?	
nonirritant	n-Hexyl bromide	?	?	
nonirritant	iso-Propyl bromide	Human data not located		
nonirritant	Di-iso-butyl ketone	Causes minor irritation to the eye (4, 20)		
nonirritant	Methyl iso-butyl ketone	?	?	
nonirritant	Allyl methacrylate	?	?	
nonirritant	Heptyl methacrylate	?	?	
nonirritant	Methyl trimethyl acetate	?	?	
nonirritant	3-Methylhexane	?	?	
nonirritant	2-Methylpentane	A human eye irritant (23)		
nonirritant	1-Methylpropyl benzene	?	?	
nonirritant	p-Methylthiobenzaldehyde	?	?	
nonirritant	Nonyl acrylate	?	?	
nonirritant	cis-Cyclo-octene	?	?	
nonirritant	n-Octyl bromide	Human data not located		

GHS Classification	Substance	CASRN	In Vivo Data Source	Substance Source	Commercial Availability	Chemical Class	Product Class	Conc. Tested	Amount Tested ¹	Purity	MW	pH	Dermal Corrosivity	# of Animals Tested	Water Solubility	Log Kow	Color
nonirritant	iso-Octylthioglycolate	25103-09-7	ECETOC	Elf Atochem, Inc.	Sigma-Aldrich Corp.	Ester, Sulfur Compound (organic)	Industrial Chemical	100%	0.1 mL	99%	204.3	n.a.	noncorrosive	3	n.a.	n.a.	clear, water-white
nonirritant	2,4-Pentanediol	625-69-4	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Alcohol	Chemical Intermediate	100%	0.1 mL	98%	104.2	n.a.	?	3	?	?	?
nonirritant	2,2-Dimethyl-3-pentanol	3970-62-5	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Alcohol	Pharmaceutical	100%	0.1 mL	97%	116.2	n.a.	noncorrosive	3	insoluble	n.a.	colorless
nonirritant	Perfluorotributylamine	311-89-7	TSCA	3M Corp.	Fisher Scientific International, Inc.	Amine	Industrial Chemical	100%	0.1 mL	80-90%	671.1	?	?	6	?	?	?
nonirritant	Phenothiazine	92-84-2	TSCA	ICI Americas, Inc.	Fisher Scientific International, Inc.	Amine, Sulfur Compound (organic)	Pesticide, Pharmaceutical Intermediate	n.a.	100 mg	99.8%	199.3	?	?	6	?	?	?
nonirritant	Phosphoric acid, tributyl ester	126-73-8	TSCA	Mobay Corp.	Sigma-Aldrich Corp.	Acid, Ester	Industrial Chemical	100%	0.1 mL	99.8%	266.3	?	?	3	?	?	?
nonirritant	Polyol 355 UCB	25791-96-2	ISOPA	Dow Europe S.A.	Dow Chemical Co. (Bulk)	Ether	Industrial Chemical	100%	0.1 mL	99.98%	n.a.	?	?	3	?	?	?
nonirritant	Polyol XZ 95435.00	52625-13-5	ISOPA	Dow Europe GmbH	Dow Chemical Co. (Bulk)	Alcohol, Ether	Industrial Chemical	100%	0.1 mL	>99.5%	530.7	?	?	3	?	?	?
nonirritant	Polyoxyethylene 23 lauryl ether (BRIJ-35)	9002-92-0	LNS	n.a.	Sigma-Aldrich Corp.	Alcohol	Pharmaceutical	10%	0.1 mL	n.a.	230.4	?	?	3	?	?	colorless
nonirritant	Potassium tetrafluoroborate	14075-53-7	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Salt (inorganic)	Industrial Chemical, Pesticide	100%	100 mg	>99%	125.9	n.a.	R34	3	4.4 g/L	n.a.	n.a.
nonirritant	3-Methoxy-1,2-propanediol	623-39-2	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Ether, Phenol	Laboratory Chemical	100%	0.1 mL	98%	106.1	?	?	3	soluble	?	?
nonirritant	(3-chloropropyl)trimethoxy-Silane	2530-87-2	TSCA	Union Carbide Corp.	Fisher Scientific International, Inc.	Ether	Industrial Chemical	100%	0.1 mL	96.3%	198.7	?	?	6	?	?	colorless to yellow
nonirritant	(3-chloropropyl)trimethoxy-Silane	2530-87-2	TSCA	Union Carbide Corp.	Fisher Scientific International, Inc.	Ether	Industrial Chemical	100%	0.1 mL	99.7%	198.7	?	?	6	?	?	colorless to yellow
nonirritant	Sodium lauryl sulfate	151-21-3	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Acid (organic) [carboxylic acid], Salt (organic)	Cleaning Agent, Cosmetic Ingredient, Food Additive, Laboratory Chemical, Pesticide Intermediate, Surfactant (anionic)	3%	0.1 mL	98%	288.4	8.0-10.0 (1% aq.)	noncorrosive	6	1 g/10 mL	1.60 (100%)	?
nonirritant	Styrene	100-42-5	ECETOC	Fisher Scientific International, Inc.	Sigma-Aldrich Corp.	Hydrocarbon (cyclic)	Chemical Intermediate, Industrial Chemical	100%	0.1 mL	99%	104.2	?	?	4	insoluble	?	colorless
nonirritant	Thiodiglycol	111-48-8	ECETOC	Fluka, Inc.	Sigma-Aldrich Corp.	Alcohol, Sulfur Compound (organic)	Industrial Chemical	100%	0.1 mL	99.8%	122.2	?	?	3	?	-0.75	?
nonirritant	Toluene	108-88-3	ECETOC	Fisher Scientific International, Inc.	Sigma-Aldrich Corp.	Hydrocarbon (cyclic)	Chemical Intermediate, Industrial Chemical, Laboratory Chemical	100%	0.1 mL	99%	92.1	?	?	4	?	?	colorless
nonirritant	3-Ethyl toluene	620-14-4	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Hydrocarbon (cyclic)	Industrial Chemical, Laboratory Chemical	100%	0.1 mL	99%	120.2	?	?	6	?	?	?
nonirritant	Triethoxyoctylsilane	2943-75-1	TSCA	Union Carbide Corp.	Fisher Scientific International, Inc.	Organosilicon Compound	Industrial Chemical	100%	0.1 mL	97.3%	276.5	?	?	6	?	?	?
nonirritant	Trifluoroethyl methacrylate	392-68-7	ECETOC	Elf Atochem, Inc.	Elf Atochem, Inc. (Bulk)	Ester	Industrial Chemical	100%	0.1 mL	99.9%	n.a.	?	?	3	?	?	?
nonirritant	Triton X-100	9002-93-1	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Ether	Surfactant (nonionic)	1%	0.1 mL	98%	250.4	7.2	noncorrosive	6	soluble	n.a.	colorless
nonirritant	Tween 20	9005-64-5	ECETOC	Sigma-Aldrich Corp.	Sigma-Aldrich Corp.	Ester, Ether	Food Additive, Laboratory Chemical, Pesticide Intermediate, Surfactant (nonionic)	100%	0.1 mL	98%	1227.5	n.a.	noncorrosive	4	100 g/L	n.a.	?
nonirritant	Xylene	1330-20-7	ECETOC	Fisher Scientific International, Inc.	Sigma-Aldrich Corp.	Hydrocarbon (cyclic)	Industrial Chemical, Laboratory Chemical, Pharmaceutical Intermediate, Solvent	100%	0.1 mL	99%	107.2	?	?	4	?	?	?
nonirritant	Xylene	1330-20-7	ECETOC	Fisher Scientific International, Inc.	Sigma-Aldrich Corp.	Hydrocarbon (cyclic)	Industrial Chemical, Laboratory Chemical, Pharmaceutical Intermediate, Solvent	100%	0.1 mL	99%	107.2	?	?	4	?	?	?

GHS Classification	Substance	Physical Form Tested	MMAS score	Corneal score	Irital score	Conjunctival score	NICEATM Category 1 SubClass.2	Tested in BCOP	Tested in HET-CAM	Tested in ICE	Tested in IRE	EPA Classification	EU Classification	FHSA Classification
nonirritant	iso-Octylthioglycolate	liquid	4.0	-	-	-	-	-	-	-	-	Category IV	nonirritant	SCNM
nonirritant	2,4-Pentandiol	liquid	4.7	-	-	-	-	-	-	-	-	Category IV	nonirritant	SCNM
nonirritant	2,2-Dimethyl-3-pentanol	liquid	8.3	-	-	-	-	-	-	-	-	Category III	nonirritant	SCNM
nonirritant	Perfluorotributylamine	liquid	0.0	-	-	-	-	-	-	-	-	Category IV	nonirritant	nonirritant
nonirritant	Phenothiazine	solid	0.0	-	-	-	-	-	-	-	-	Category IV	nonirritant	nonirritant
nonirritant	Phosphoric acid, tributyl ester	liquid	13.3	-	-	-	-	-	-	-	-	Category III	nonirritant	Insufficient Animal Data
nonirritant	Polyol 355 UCB	liquid	0.0	-	-	-	-	-	-	-	-	Category IV	nonirritant	SCNM
nonirritant	Polyol XZ 95435.00	liquid	0.0	-	-	-	-	-	-	-	-	Category IV	nonirritant	SCNM
nonirritant	Polyoxyethylene 23 lauryl ether (BRIJ-35)	liquid	0.0	-	-	-	-	-	X	-	-	Category IV	nonirritant	nonirritant
nonirritant	Potassium tetrafluoroborate	solid	0.0	-	-	-	-	-	-	-	-	Category IV	nonirritant	SCNM
nonirritant	3-Methoxy-1,2-propanediol	liquid	0.0	-	-	-	-	-	-	-	-	Category IV	nonirritant	SCNM
nonirritant	(3-chloropropyl)trimethoxy-Silane	liquid	0.3	-	-	-	-	-	-	-	-	Category IV	nonirritant	nonirritant
nonirritant	(3-chloropropyl)trimethoxy-Silane	liquid	0.0	-	-	-	-	-	-	-	-	Category IV	nonirritant	nonirritant
nonirritant	Sodium lauryl sulfate	liquid	7.3	-	-	-	-	X	X	X	X	Category III	nonirritant	irritant
nonirritant	Styrene	liquid	6.8	-	-	-	-	-	-	-	-	Category III	nonirritant	SCNM
nonirritant	Thiodiglycol	liquid	5.3	-	-	-	-	-	-	-	-	Category III	nonirritant	SCNM
nonirritant	Toluene	liquid	9.0	-	-	-	-	-	X	X	X	Category III	nonirritant	SCNM
nonirritant	3-Ethyl toluene	liquid	2.3	-	-	-	-	-	-	-	-	Category IV	nonirritant	nonirritant
nonirritant	Triethoxyoctylsilane	liquid	2.7	-	-	-	-	-	-	-	-	Category IV	nonirritant	nonirritant
nonirritant	Trifluoroethyl methacrylate	liquid	2.7	-	-	-	-	-	-	-	-	Category IV	nonirritant	SCNM
nonirritant	Triton X-100	liquid	1.7	-	-	-	-	X	-	-	-	Category II	R36	irritant
nonirritant	Tween 20	liquid	40.0	-	-	-	-	X	X	X	X	Category III	nonirritant	SCNM
nonirritant	Xylene	liquid	1.5	-	-	-	-	X	-	-	-	Category IV	nonirritant	SCNM
nonirritant	Xylene	liquid	9.0	-	-	-	-	-	-	-	-	Category II	nonirritant	SCNM

GHS Classification	Substance	Human Exposure Summary	Animal Exposure Summary for Category 1(H) Substances	Notes
nonirritant	iso-Octylthioglycolate	Human data not located		
nonirritant	2,4-Pentandiol	Human data not located		
nonirritant	2,2-Dimethyl-3-pentanol	Human data not located		
nonirritant	Perfluorotributylamine	?	?	
nonirritant	Phenothiazine	?	?	
nonirritant	Phosphoric acid, tributyl ester	?	?	
nonirritant	Polyol 355 UCB	?	?	
nonirritant	Polyol XZ 95435.00	?	?	
nonirritant	Polyoxyethylene 23 lauryl ether (BRIJ-35)	?	?	
nonirritant	Potassium tetrafluoroborate	Human data not located		
nonirritant	3-Methoxy-1,2-propanediol	Human data not located		
nonirritant	(3-chloropropyl)trimethoxy-Silane	?	?	
nonirritant	(3-chloropropyl)trimethoxy-Silane	?	?	
nonirritant	Sodium lauryl sulfate	Sodium lauryl sulfate is said to have been the commonest cause of eye irritation by commercial shampoos (10)		
nonirritant	Styrene	?	?	
nonirritant	Thiodiglycol	?	?	
nonirritant	Toluene	Vapors of toluene cause noticeable sensation of irritation to human eyes at 300-440 ppm in air, but even at 800 ppm, irritation is slight. Vapors irritate eyes and upper respiratory tract; liquid irritates eyes (10, 27).		
nonirritant	3-Ethyl toluene	?	?	
nonirritant	Triethoxyoctylsilane	?	?	
nonirritant	Trifluoroethyl methacrylate	?	?	
nonirritant	Triton X-100	Human data not located		
nonirritant	Tween 20	Human data not located		
nonirritant	Xylene	?	?	
nonirritant	Xylene	?	?	

Please see abbreviations and references in **Appendix V-A1**