

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
1-1 (#1)	-	liquid	n.p.	100%	n.p.	-							83.6			Severe	Severe	Swanson and Harbell (2000)
1-2 (#2)	-	liquid	n.p.	100%	n.p.	-							12.4			Mild	Mild	Swanson and Harbell (2000)
1-3 (#3)	-	liquid	n.p.	100%	n.p.	-							29.6			Moderate	Moderate	Swanson and Harbell (2000)
2-4 (#4)	-	liquid	n.p.	100%	n.p.	-							7.3			Mild	Mild	Swanson and Harbell (2000)
2-7 (#7)	-	liquid	n.p.	100%	n.p.	-							21.4			Moderate	Moderate	Swanson and Harbell (2000)
2-8 (#8)	-	liquid	n.p.	100%	n.p.	-							31.8			Moderate	Moderate	Swanson and Harbell (2000)
Acetone	67-64-1	liquid	water soluble	100%	99	1	90.3			3.676			145.5			Very severe		Balls et al. (1995)
Acetone	67-64-1	liquid	water soluble	100%	99	2	83.7			2.389			119.5			Very severe		Balls et al. (1995)
Acetone	67-64-1	liquid	water soluble	100%	99	3	55.7			4.315			120.4			Very severe	Very Severe	Balls et al. (1995)
Acetone	67-64-1	liquid	water soluble	100%	99	4	94.33			2.492			131.72			Very severe		Balls et al. (1995)
Acetone	67-64-1	liquid	water soluble	100%	99	5	69.3			1.942			98.4			Very severe		Balls et al. (1995)
Acetone	67-64-1	liquid	water soluble	100%	n.p.	-	1.38			0.653						Severe	Severe	Casterton et al. (1996)
Alkyl phosphoric acid ester/amine salt	-	liquid	moderate	100%	n.p.	-	37.7			3.577			91.3			Severe	Severe	Bailey et al. (2004)
All Purpose Cleaner (#5)	-	liquid	n.p.	100%	n.p.	-	102.5	5		1.252	5		121.3	5		Severe	Severe	Swanson et al. (1995)
All Purpose Cleaner (#7)	-	liquid	n.p.	100%	n.p.	-	348.1	5		3.013	5		393.3	5		Severe	Severe	Swanson et al. (1995)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	1							156			Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	2							138			Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	3							232			Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	4							156			Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	5							132			Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	6							191			Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	7							190			Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	8							166			Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	9	94.1	6	18.9	1.948	6	0.455	123	6	14.4	Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	10							101			Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	11							200			Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	12							90			Severe		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	1							5			Mild		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	2							4			Mild		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	3							10			Mild		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	4							3			Mild		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	5							5			Mild		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	6							28			Moderate		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	7							2			Mild		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	8							4			Mild		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	9	9.7	6	2.3	0.012	6	0.007	10	6	2.3	Mild		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	10							6			Mild		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	11							2			Mild		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	12							2			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	1							7			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	2							5			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	3							3			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	4							5			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	5							6			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	6							7			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	7							5			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	8							6			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	9	10.9	6	1.4	0.144	6	0.188	13	6	2.5	Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	10							11			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	11							5			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	12							11			Mild		Gautheron et al. (1994)
Ammonium nitrate	6484-52-2	solid	water soluble	20%	>99.9	1	6.3			0.132			8.3			Mild		Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	water soluble	20%	>99.9	2	6			0.026			6.4			Mild		Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	water soluble	20%	>99.9	3	6			0.079			7.2			Mild		Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	water soluble	20%	>99.9	4	11.34			0.698			21.82			Mild		Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	water soluble	20%	>99.9	5	4.7			0.034			5.2			Mild		Balls et al. (1995)

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Ammonium nitrate	6484-52-2	n.p.	n.p.	100%	n.p.	1 (1)	4.3	3	2.1	0.037	3	0.036	4.9	3	2.4	Mild	Mild	Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	n.p.	100%	n.p.	1 (2)	5.0	3	1.2	0.059	3	0.031	5.9	3	1.4	Mild	Mild	Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	n.p.	100%	n.p.	2 (1)	1.6	3	1.2	0.153	3	0.059	3.9	3	1.8	Mild	Mild	Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	n.p.	100%	n.p.	2 (2)	2.0	3	0.6	0.107	3	0.044	3.6	3	1	Mild	Mild	Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	n.p.	100%	n.p.	3 (1)	3.7	3	0.6	0.100	3	0.033	5.2	3	0.6	Mild	Mild	Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	n.p.	100%	n.p.	3 (2)	4.3	3	0.6	0.158	3	0.07	6.7	3	1.5	Mild	Mild	Southee (1998)
Amway all fabric bleach	-	n.p.	n.p.	100%	n.p.	-	0.400			1.435						Severe	Severe	Casterton et al. (1996)
Amway automatic dishwashing compound for soft water	-	n.p.	n.p.	100%	n.p.	-	2.249			1.381						Severe	Severe	Casterton et al. (1996)
Amway automatic dishwashing compound, standard formula	-	n.p.	n.p.	100%	n.p.	-	0.683			0.477						Moderate	Moderate	Casterton et al. (1996)
Amway concrete floor cleaner	-	n.p.	n.p.	100%	n.p.	-	2.205			1.839						Severe	Severe	Casterton et al. (1996)
Amway Dish Drops dishwashing liquid	-	n.p.	n.p.	100%	n.p.	-	0.290			0.493						Moderate	Moderate	Casterton et al. (1996)
Amway dry chlorine bleach	-	n.p.	n.p.	100%	n.p.	-	0.204			0.311						Moderate	Moderate	Casterton et al. (1996)
Amway fabric softener	-	n.p.	n.p.	100%	n.p.	-	0.089			0.013						Mild	Mild	Casterton et al. (1996)
Amway Kool Wash delicate fabric detergent	-	n.p.	n.p.	100%	n.p.	-	0.039			0.326						Moderate	Moderate	Casterton et al. (1996)
Amway LOC all purpose cleaner	-	n.p.	n.p.	100%	n.p.	-	0.193			0.050						Mild	Mild	Casterton et al. (1996)
Amway prewash liquid	-	liquid	n.p.	100%	n.p.	-	0.142			0.079						Mild	Mild	Casterton et al. (1996)
Amway Pursue disinfectant cleaner	-	n.p.	n.p.	100%	n.p.	-	1.437			0.763						Severe	Severe	Casterton et al. (1996)
Amway Redu dye stain remover	-	n.p.	n.p.	100%	n.p.	-	0.138			0.028						Mild	Mild	Casterton et al. (1996)
Amway SA8 laundry liquid	-	liquid	n.p.	100%	n.p.	-	0.032			0.179						Moderate	Moderate	Casterton et al. (1996)
Amway SA8 limited phos laundry powder	-	solid	n.p.	100%	n.p.	-	0.415			0.285						Moderate	Moderate	Casterton et al. (1996)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	1							-2			Nonirritant	Mild	Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	2							1			Mild	Mild	Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	3							-3			Nonirritant	Mild	Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	4							0			Mild	Mild	Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	5							0			Mild	Mild	Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	6							-1			Nonirritant	Mild	Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	7							0			Mild	Mild	Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	8							0			Mild	Mild	Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	9	1.4	6	1.2	0.003	6	0.007	1	6	1.3	Mild	Mild	Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	10							0			Mild	Mild	Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	11							-2			Nonirritant	Mild	Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	12							2			Mild	Mild	Gautheron et al. (1994)
Anti-Dandruff Shampoo (HZY)	-	n.p.	n.p.	100%	n.p.	-	0.092			0.182						Moderate	Moderate	Casterton et al. (1996)
Anti-Dandruff Shampoo (HZY) 100%	-	n.p.	n.p.	10%	n.p.	-				0.847	3	0.199	20.8			Severe	Severe	Gettings et al. (1996)
Aromatic hydrocarbon #1	-	liquid	negligible	100%	n.p.	-	2.7			0.000			2.7			Mild	Mild	Bailey et al. (2004)
Aromatic hydrocarbon #2	-	liquid	negligible	100%	n.p.	-	4.3			0.017			4.6			Mild	Mild	Bailey et al. (2004)
Arvl phosphonates	-	liquid	moderate	100%	n.p.	-	20.3			1.399			41.3			Moderate	Moderate	Bailey et al. (2004)
L-Aspartic acid	70-47-3	solid	water soluble	20%	100	1	2			-0.011			1.8			Mild	Mild	Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	water soluble	20%	100	2	1.7			-0.107			0.1			Mild	Mild	Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	water soluble	20%	100	3	2.7			-0.003			2.6			Mild	Mild	Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	water soluble	20%	100	4	0.33			0.03			0.788			Mild	Mild	Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	water soluble	20%	100	5	0			0.082			1.2			Mild	Mild	Balls et al. (1995)
Baby Shampoo No. 1 (HZP)	-	n.p.	n.p.	100%	n.p.	-	-0.02			0.062						Mild	Mild	Casterton et al. (1996)
Baby Shampoo No. 1 (HZP) 100%	-	n.p.	n.p.	10%	n.p.	-				0.261	3	0.05	4.0			Nonsevere	Nonsevere	Gettings et al. (1996)
Baby Shampoo No. 2 (HZF)	-	n.p.	n.p.	100%	n.p.	-	0.067			0.265						Moderate	Moderate	Casterton et al. (1996)
Baby Shampoo No. 2 (HZF) 100%	-	n.p.	n.p.	10%	n.p.	-				0.425	3	0.082	8.3			Nonsevere	Nonsevere	Gettings et al. (1996)
Bathroom Cleaner (#6)	-	liquid	n.p.	100%	n.p.	-	64	5		0.95	5		78.3	5		Severe	Severe	Swanson et al. (1995)
Benchmark-Group 1 (#12)	-	liquid	n.p.	100%	n.p.	-							60.1			Severe	Severe	Swanson and Harbell (2000)
Benchmark-Group 2 (#13)	-	liquid	n.p.	100%	n.p.	-							60.1			Severe	Severe	Swanson and Harbell (2000)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	1 (1)	84.0	3	3.8	7.408	3	0.903	195.2	3	11.3	Very severe	Very severe	Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	1 (2)	85.6	3	3.2	3.305	3	0.225	135.2	3	5.2	Very severe	Very severe	Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	1 (3)	82.0	3	1.7	3.729	3	0.25	137.9	3	2.3	Very severe	Very severe	Southee (1998)

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Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	1 (4)	85.0	3	5.2	4.766	3	1.132	156.5	3	18.6	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	1 (5)	87.7	3	1.7	3.354	3	0.108	138.0	3	0.1	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	1 (6)	91.7	3	7.0	5.67	3	1.096	176.8			Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	1 (7)	98.3	3	2.6	5.645	3	0.523	183.0			Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	1 (8)	87.7	3	2.9	5.848	3	0.581	175.4			Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	2 (1)	88.0	3	7.5	4.426	3	0.623	154.4	3	11.1	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	2 (2)	94.6	3	10.4	4.148	3	0.662	156.9	3	18.6	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	2 (3)	87.0	3	7.5	4.252	3	0.069	150.8	3	7.1	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	2 (4)	93.0	3	3.0	4.278	3	1.058	157.2	3	18.0	Very severe	Very Severe	Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	2 (5)	98.3	3	2.3	3.972	3	0.360	157.9	3	3.4	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	2 (6)	95.7	3	5.0	4.129	3	0.581	157.0			Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	2 (7)	98.0	3	5.1	4.144	3	0.232	160.2			Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	3 (1)	96.7	3	2.0	4.015	3	1.011	156.9	3	17.1	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	3 (2)	92.6	3	11.8	4.719	3	1.547	163.4	3	16.2	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	3 (3)	105.0	3	6.1	4.316	3	0.320	169.7	3	10.2	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	3 (4)	95.3	3	4.0	4.497	3	1.007	162.8	3	11.4	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	3 (5)	92.3	3	7.2	3.948	3	0.231	151.6	3	7.7	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	3 (6)	93.7	3	4.9	4.624	3	1.708	163.1	3	22.1	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	3 (7)	100.7	3	2.5	4.473	3	0.619	167.8	3	7.8	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	3 (8)	96.7	3	2.0	9.016	3	1.011	156.9	3	17.1	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	3 (9)	97.3	3	5.1	4.183	3	0.514	160.0	3	8.2	Very severe		Southee (1998)
Benzalkonium chloride (1 %)	8001-54-5	liquid	surfactant	1%	98	1	59			3.588			112.8			Very severe		Balls et al. (1995)
Benzalkonium chloride (1 %)	8001-54-5	liquid	surfactant	1%	98	2	37			3.566			90.5			Very severe		Balls et al. (1995)
Benzalkonium chloride (1 %)	8001-54-5	liquid	surfactant	1%	98	3	34.3			4.336			99.4			Very severe	Very Severe	Balls et al. (1995)
Benzalkonium chloride (1 %)	8001-54-5	liquid	surfactant	1%	98	4	22			2.699			62.49			Severe		Balls et al. (1995)
Benzalkonium chloride (1 %)	8001-54-5	liquid	surfactant	1%	98	5	38			2.706			78.6			Severe		Balls et al. (1995)
Benzalkonium chloride (1%)	8001-54-5	liquid	surfactant	1%	n.p.	-	0.970			0.764						Severe	Severe	Casterton et al. (1996)
Benzalkonium chloride (10%)	8001-54-5	liquid	surfactant	10%	98	1	75.3			4.456			142.2			Very severe		Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	surfactant	10%	98	2	79.3			5.223			157.7			Very severe		Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	surfactant	10%	98	3	61.7			4.142			123.8			Very severe	Very Severe	Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	surfactant	10%	98	4	63			4.967			137.5			Very severe		Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	surfactant	10%	98	5	74.7			3.096			121.1			Very severe		Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	surfactant	10%	n.p.	-	1.612			1.180						Severe	Severe	Casterton et al. (1996)
Benzalkonium chloride (5%)	8001-54-5	liquid	surfactant	5%	98	1	126.6			3.264			126.6			Very severe		Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	surfactant	5%	98	2	163.7			6.599			163.7			Very severe		Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	surfactant	5%	98	3	110.7			3.891			110.7			Very severe	Very Severe	Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	surfactant	5%	98	4	130.41			4.338			130.41			Very severe		Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	surfactant	5%	98	5	111.1			3.117			111.1			Very severe		Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	surfactant	5%	n.p.	-	1.332			0.776						Severe	Severe	Casterton et al. (1996)
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	1							128			Severe		Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	2							124			Severe		Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	3							163			Severe		Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	4							106			Severe		Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	5							128			Severe		Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	6							129			Severe		Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	7							142			Severe		Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	8							129			Severe		Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	9	84.6	6	3.3	5.42	6	0.949	166	6	14.5	Severe		Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	11							142			Severe		Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	12							116			Severe		Gautheron et al. (1994)
Benzoyl-L-tartaric acid	2743-38-6	solid	water insoluble	20%	-	1	169.7			0.218			173			Very severe		Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	solid	water insoluble	20%	-	2	286.7			0.134			288.7			Very severe		Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	solid	water insoluble	20%	-	3	90			0.073			91.1			Very severe	Very Severe	Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	solid	water insoluble	20%	-	4	147			0.191			149.86			Very severe		Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	solid	water insoluble	20%	-	5	141.3			0.266			145.3			Very severe		Balls et al. (1995)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	1							4			Mild		Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	2							1			Mild		Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	3							0			Mild		Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	4							1			Mild		Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	5							1			Mild		Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	6							3			Mild		Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	7							1			Mild		Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	8							-10			Nonirritant		Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	9	3.1	6	2.3	0.029	6	0.014	4	6	2.2	Mild		Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	10							-1			Nonirritant		Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	11							1			Mild		Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	12							6			Mild		Gautheron et al. (1994)
BRU-35	9002-92-0	surfactant	n.p.	10%	n.p.	1							0			Mild		Gautheron et al. (1994)
BRU-35	9002-92-0	surfactant	n.p.	10%	n.p.	2							2			Mild		Gautheron et al. (1994)
BRU-35	9002-92-0	surfactant	n.p.	10%	n.p.	3							-1			Nonirritant		Gautheron et al. (1994)
BRU-35	9002-92-0	surfactant	n.p.	10%	n.p.	4							1			Mild		Gautheron et al. (1994)
BRU-35	9002-92-0	surfactant	n.p.	10%	n.p.	5							0			Mild		Gautheron et al. (1994)
BRU-35	9002-92-0	surfactant	n.p.	10%	n.p.	6							0			Mild		Gautheron et al. (1994)
BRU-35	9002-92-0	surfactant	n.p.	10%	n.p.	7							0			Mild		Gautheron et al. (1994)
BRU-35	9002-92-0	surfactant	n.p.	10%	n.p.	8							0			Mild		Gautheron et al. (1994)
BRU-35	9002-92-0	surfactant	n.p.	10%	n.p.	9	1.1	6	0.6	-0.002	6	0.008	1	6	0.7	Mild		Gautheron et al. (1994)
BRU-35	9002-92-0	surfactant	n.p.	10%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
BRU-35	9002-92-0	surfactant	n.p.	10%	n.p.	11							-2			Nonirritant		Gautheron et al. (1994)
BRU-35	9002-92-0	surfactant	n.p.	10%	n.p.	12							-2			Nonirritant		Gautheron et al. (1994)
4-Bromophenotole	-	n.p.	n.p.	100%	n.p.	-	0.079			0.018						Mild	Mild	Casterton et al. (1996)
Bubble Bath (HZK)	-	n.p.	n.p.	100%	n.p.	-	0.007			0.103						Moderate	Moderate	Casterton et al. (1996)
Bubble Bath (HZK) 100%	-	n.p.	n.p.	10%	n.p.	-				0.956	3	0.324	17.5			Severe	Severe	Gettings et al. (1996)
n-Butanol	71-36-3	liquid	n.p.	100%	n.p.	-	0.414			0.671						Severe	Severe	Casterton et al. (1996)
2-Butoxyethanol	111-76-2	liquid	n.p.	100%	n.p.	-	0.394			1.160						Severe	Severe	Casterton et al. (1996)
Butyl acetate	123-86-4	liquid	water insoluble*	100%	n.p.	1	9			2.7			49.5			Moderate		Balls et al. (1995)
Butyl acetate	123-86-4	liquid	water insoluble*	100%	n.p.	2	7.7			1.989			37.5			Moderate		Balls et al. (1995)
Butyl acetate	123-86-4	liquid	water insoluble*	100%	n.p.	3	5.7			2.546			43.9			Moderate	Moderate	Balls et al. (1995)
Butyl acetate	123-86-4	liquid	water insoluble*	100%	n.p.	4	5			1.257			23.86			Mild		Balls et al. (1995)
Butyl acetate	123-86-4	liquid	water insoluble*	100%	n.p.	5	2.3			1.051			18.1			Mild		Balls et al. (1995)
Butyl cellulolve	111-76-2	liquid	n.p.	100%	n.p.	1 (1)	39	3	7.8	4.625	3	0.471	108.3	3	12.9	Very severe		Southee (1998)
Butyl cellulolve	111-76-2	liquid	n.p.	100%	n.p.	1 (2)	43	3	4.0	4.589	3	0.418	111.8	3	5.5	Very severe		Southee (1998)
Butyl cellulolve	111-76-2	liquid	n.p.	100%	n.p.	2 (1)	29.6	3	1.5	4.213	3	0.78	92.8	3	13	Very severe		Southee (1998)
Butyl cellulolve	111-76-2	liquid	n.p.	100%	n.p.	2 (2)	31.3	3	2.3	4.526	3	0.864	99.2	3	10.7	Very severe		Southee (1998)
Butyl cellulolve	111-76-2	liquid	n.p.	100%	n.p.	3 (1)	37.7	3	1.0	3.813	3	0.933	94.9	3	13.8	Very severe		Southee (1998)
Butyl cellulolve	111-76-2	liquid	n.p.	100%	n.p.	3 (2)	37.7	3	6.1	4.031	3	1.206	98.2	3	21.6	Very severe		Southee (1998)
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	1							48			Moderate		Gautheron et al. (1994)
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	2							44			Moderate		Gautheron et al. (1994)
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	3							64			Severe		Gautheron et al. (1994)
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	4							35			Moderate		Gautheron et al. (1994)
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	5							35			Moderate		Gautheron et al. (1994)
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	6							30			Moderate		Gautheron et al. (1994)
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	7							80			Severe		Gautheron et al. (1994)
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	8							32			Moderate		Gautheron et al. (1994)
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	9	34.2	6	3.1	0.495	6	0.199	42	6	5	Moderate		Gautheron et al. (1994)
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	10							53			Moderate		Gautheron et al. (1994)
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	11							35			Moderate		Gautheron et al. (1994)
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	12							49			Moderate		Gautheron et al. (1994)
gamma-Butyrolactone	96-48-0	liquid	water soluble	100%	>99	1	37.3			3.553			90.6			Very severe		Balls et al. (1995)
gamma-Butyrolactone	96-48-0	liquid	water soluble	100%	>99	2	22.7			0.682			32.9			Moderate		Balls et al. (1995)
gamma-Butyrolactone	96-48-0	liquid	water soluble	100%	>99	3	22			0.63			31.5			Moderate		Balls et al. (1995)
gamma-Butyrolactone	96-48-0	liquid	water soluble	100%	>99	4	48.67			2.192			81.55			Very severe		Balls et al. (1995)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference	
gamma-Butyrolactone	96-48-0	liquid	water soluble	100%	>99	5	31.7			2.357			67.1			Severe		Balls et al. (1995)	
Captan 90 concentrate	133-06-2	solid	water soluble	20%	20%	90	1	28		-0.008			27.8			Moderate		Balls et al. (1995)	
Captan 90 concentrate	133-06-2	solid	water soluble	20%	20%	90	2	26.3		0.055			27.2			Moderate		Balls et al. (1995)	
Captan 90 concentrate	133-06-2	solid	water soluble	20%	20%	90	3	34.7		0.007			34.8			Moderate	Moderate	Balls et al. (1995)	
Captan 90 concentrate	133-06-2	solid	water soluble	20%	20%	90	4	102		0.061			102.918			Very severe		Balls et al. (1995)	
Captan 90 concentrate	133-06-2	solid	water soluble	20%	20%	90	5	26.3		0.004			26.4			Moderate		Balls et al. (1995)	
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	20%	95	1	97.3		0.02			97.6			Very severe		Balls et al. (1995)	
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	20%	95	2	96.3		0.116			98.1			Very severe		Balls et al. (1995)	
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	20%	95	3	57.3		0.012			57.5			Severe	Severe	Balls et al. (1995)	
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	20%	95	4	64		0.022			64.33			Severe		Balls et al. (1995)	
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	20%	95	5	72		0.128			73.9			Severe		Balls et al. (1995)	
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	100%	n.p.	-	0.331			0.002						Mild	Mild	Casterton et al. (1996)	
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	20%	95	1 (1)	53.7	3	4.6	0.012	3	0.012	53.9	3	4.9	Moderate		Southee (1998)
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	20%	95	1 (2)	47.7	3	3.5	0.002	3	0.02	47.7	3	3.4	Moderate		Southee (1998)
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	20%	95	2 (1)	46.3	3	3.2	0.05	3	0.021	47.1	3	3.1	Moderate		Southee (1998)
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	20%	95	2 (2)	46.4	3	2.9	0.058	3	0.014	47.2	3	2.9	Moderate		Southee (1998)
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	20%	95	3 (1)	42	3	4.5	0.013	3	0.016	42.2	3	4.3	Moderate		Southee (1998)
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	20%	95	3 (2)	41.3	3	4.0	0.035	3	0.006	41.8	3	3.9	Moderate		Southee (1998)
Carboxylic acid amides	-	solid	moderate	100%	n.p.	-	10.7			1.125			27.5			Moderate	Moderate	Bailey et al. (2004)	
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	surfactant	0.10%	n.p.	98	1	6.7		0.293			11			Mild		Balls et al. (1995)	
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	surfactant	0.10%	n.p.	98	2	1.7		0.163			4.1			Mild		Balls et al. (1995)	
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	surfactant	0.10%	n.p.	98	3	3		0.606			12.1			Mild	Mild	Balls et al. (1995)	
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	surfactant	0.10%	n.p.	98	4	3.33		0.066			4.33			Mild		Balls et al. (1995)	
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	surfactant	0.10%	n.p.	98	5	6.3		0.543			14.5			Mild		Balls et al. (1995)	
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	surfactant	0%	n.p.	-	0.082			0.089						Mild	Mild	Casterton et al. (1996)	
Cetylpyridinium bromide (1%)	140-72-7	liquid	surfactant	1%	n.p.	-	0.425			0.364						Moderate	Moderate	Casterton et al. (1996)	
Cetylpyridinium bromide (10%)	140-72-7	liquid	surfactant	10%	n.p.	98	1	22.7		1.389			43.5			Moderate		Balls et al. (1995)	
Cetylpyridinium bromide (10%)	140-72-7	liquid	surfactant	10%	n.p.	98	2	27.7		4.128			89.6			Very severe		Balls et al. (1995)	
Cetylpyridinium bromide (10%)	140-72-7	liquid	surfactant	10%	n.p.	98	3	24.7		3.759			81			Very severe	Very Severe	Balls et al. (1995)	
Cetylpyridinium bromide (10%)	140-72-7	liquid	surfactant	10%	n.p.	98	4	17		3.97			71.22			Severe		Balls et al. (1995)	
Cetylpyridinium bromide (10%)	140-72-7	liquid	surfactant	10%	n.p.	98	5	23		3.58			76.7			Severe		Balls et al. (1995)	
Cetylpyridinium bromide (10%)	140-72-7	liquid	surfactant	10%	n.p.	-	0.855			0.705						Severe	Severe	Casterton et al. (1996)	
Cetylpyridinium bromide (6%)	140-72-7	liquid	surfactant	6%	n.p.	98	1	31.7		2.705			72.2			Severe		Balls et al. (1995)	
Cetylpyridinium bromide (6%)	140-72-7	liquid	surfactant	6%	n.p.	98	2	38.3		3.195			86.3			Very severe		Balls et al. (1995)	
Cetylpyridinium bromide (6%)	140-72-7	liquid	surfactant	6%	n.p.	98	3	18.3		3.015			63.6			Severe	Severe	Balls et al. (1995)	
Cetylpyridinium bromide (6%)	140-72-7	liquid	surfactant	6%	n.p.	98	4	25.33		2.892			68.72			Severe		Balls et al. (1995)	
Cetylpyridinium bromide (6%)	140-72-7	liquid	surfactant	6%	n.p.	98	5	34		2.097			65.4			Severe		Balls et al. (1995)	
Cetylpyridinium bromide (6%)	140-72-7	liquid	surfactant	6%	n.p.	-	0.908			0.775						Severe	Severe	Casterton et al. (1996)	
Chlorhexidine	55-56-1	solid	water insoluble*	20%	n.p.	1	141			0.399			147			Very severe		Balls et al. (1995)	
Chlorhexidine	55-56-1	solid	water insoluble*	20%	n.p.	2	124			-0.071			122.9			Very severe		Balls et al. (1995)	
Chlorhexidine	55-56-1	solid	water insoluble*	20%	n.p.	3	96.3			0.062			97.3			Very severe	Very Severe	Balls et al. (1995)	
Chlorhexidine	55-56-1	solid	water insoluble*	20%	n.p.	4	97.66			0.277			101.78			Very severe		Balls et al. (1995)	
Chlorhexidine	55-56-1	solid	water insoluble*	20%	n.p.	5	98.7			0.189			101.5			Very severe		Balls et al. (1995)	
2-Chloro-2,4,4-trimethylpentane	-	liquid	negligible	100%	n.p.	-	4.0			0.004			4.1			Mild	Mild	Bailey et al. (2004)	
Clarified slurry oil	-	liquid	negligible	100%	n.p.	-	2.3			0.000			2.3			Mild	Mild	Bailey et al. (2004)	
Cleaner/Degreaser (#13)	-	liquid	n.p.	100%	n.p.	-	314.3	5		2.623	5		353.6	5		Severe	Severe	Swanson et al. (1995)	
Cleansing Gel (HZQ)	-	n.p.	n.p.	100%	n.p.	-	0.034			0.073						Mild	Mild	Casterton et al. (1996)	
Cleansing Gel (HZQ) 100%	-	n.p.	n.p.	10%	n.p.	-				0.164	3	0.05	2.3			Nonsevere	Nonsevere	Gettings et al. (1996)	
Cutting fluid (conc.) #1	-	liquid	emulsifies	100%	n.p.	-	3.3			0.001			3.5			Mild	Mild	Bailey et al. (2004)	
Cutting fluid (conc.) #2	-	liquid	emulsifies	100%	n.p.	-	4.3			0.038			4.9			Mild	Mild	Bailey et al. (2004)	
Cyclohexanol	108-93-0	liquid	water soluble	100%	n.p.	1	18.3			4.442			85			Very severe		Balls et al. (1995)	
Cyclohexanol	108-93-0	liquid	water soluble	100%	n.p.	2	7.3			2.838			49.9			Moderate		Balls et al. (1995)	
Cyclohexanol	108-93-0	liquid	water soluble	100%	n.p.	3	12			3.87			70.1			Severe	Moderate	Balls et al. (1995)	
Cyclohexanol	108-93-0	liquid	water soluble	100%	n.p.	4	11.66			2.71			52.24			Moderate		Balls et al. (1995)	
Cyclohexanol	108-93-0	liquid	water soluble	100%	n.p.	5	7			2.392			43.2			Moderate		Balls et al. (1995)	
Cyclohexanol	108-93-0	liquid	water soluble	100%	n.p.	-	0.312			0.647						Severe	Severe	Casterton et al. (1996)	

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	1							92			Severe		Gautheron et al. (1994)
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	2							108			Severe		Gautheron et al. (1994)
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	3							96			Severe		Gautheron et al. (1994)
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	4							81			Severe		Gautheron et al. (1994)
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	5							130			Severe		Gautheron et al. (1994)
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	6							93			Severe		Gautheron et al. (1994)
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	7							104			Severe		Gautheron et al. (1994)
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	8							90			Severe		Gautheron et al. (1994)
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	9	76.6	6	3.9	4.341	6	0.551	142	6	8.2	Severe		Gautheron et al. (1994)
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	11							118			Severe		Gautheron et al. (1994)
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	12							108			Severe		Gautheron et al. (1994)
Degreaser (#16)	-	liquid	n.p.	100%	n.p.	-	225.4	5		2.022	5		255.7	5		Severe	Severe	Swanson et al. (1995)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	1							96			Severe		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	2							72			Severe		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	3							106			Severe		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	4							73			Severe		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	5							119			Severe		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	6							103			Severe		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	7							88			Severe		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	8							46			Moderate		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	9	13.9	6	2.6	5.718	6	0.511	100	6	8	Severe		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	10							60			Severe		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	11							200			Severe		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	12							59			Severe		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	1							53			Moderate		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	2							41			Moderate		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	3							105			Severe		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	4							39			Moderate		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	5							42			Moderate		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	6							34			Moderate		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	7							49			Moderate		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	8							41			Moderate		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	9	31.1	6	3.2	4.119	6	1.341	92	6	22	Severe		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	11							36			Moderate		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	12							56			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	1							104			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	2							134			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	3							82			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	4							118			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	5							110			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	6							66			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	7							88			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	8							193			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	9	75.2	6	14.2	0.416	6	0.116	82	6	13.7	Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	11							213			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	12							135			Severe		Gautheron et al. (1994)
Dibenzyl phosphate	1623-08-1	solid	water insoluble*	20%	99	1	304.3			-0.017			304.1			Very severe		Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	water insoluble*	20%	99	2	389.3			0.117			391.1			Very severe		Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	water insoluble*	20%	99	3	418			-0.002			418			Very severe		Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	water insoluble*	20%	99	4	467			-0.016			467.09			Very severe		Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	water insoluble*	20%	99	5	304			0.234			307.5			Very severe		Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	water insoluble*	100%	99	1	9			0.058			9.9			Mild		Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	water insoluble*	100%	99	2	10.3			0.059			11.2			Mild		Balls et al. (1995)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	water insoluble*	100%	99	3	9.7			0.078			10.8			Mild	Mild	Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	water insoluble*	100%	99	4	14.33			0.007			14.43			Mild	Mild	Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	water insoluble*	100%	99	5	5.4			0.012			5.6			Mild	Mild	Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	water insoluble*	100%	n.p.	-	0.124			0.106						Mild	Mild	Casteron et al. (1996)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	1							23			Mild	Mild	Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	2							23			Mild	Mild	Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	3							18			Mild	Mild	Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	4							28			Moderate	Mild	Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	5							16			Mild	Mild	Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	6							31			Moderate	Mild	Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	7							18			Mild	Mild	Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	8							71			Severe	Mild	Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	9	19.3	6	4.8	-0.01	6	0.004	19	6	4.7	Mild	Mild	Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	10							20			Mild	Mild	Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	11							34			Moderate	Mild	Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	12							14			Mild	Mild	Gautheron et al. (1994)
2,4-Difluoronitrobenzene	446-35-5	liquid	n.p.	100%	n.p.	-	0.049			0.008						Mild	Mild	Casteron et al. (1996)
1,3-Diisopropylbenzene	99-62-7	liquid	n.p.	100%	n.p.	-	0.029			0.000						Mild	Mild	Casteron et al. (1996)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	1							0			Mild	Mild	Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	2							3			Mild	Mild	Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	3							1			Mild	Mild	Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	4							3			Mild	Mild	Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	5							1			Mild	Mild	Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	6							5			Mild	Mild	Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	7							3			Mild	Mild	Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	8							1			Mild	Mild	Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	9	0.7	6	1.8	0.097	6	0.176	2	6	2.6	Mild	Mild	Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	10							no data			n.a.	Mild	Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	11							5			Mild	Mild	Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	12							8			Mild	Mild	Gautheron et al. (1994)
2,2-Dimethylbutanoic acid	595-37-9	liquid	water insoluble	100%	96	1	65			2.583			103.8			Very severe	Very Severe	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	water insoluble	100%	96	2	58.3			3.78			115			Very severe	Very Severe	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	water insoluble	100%	96	3	62.7			4.601			131.7			Very severe	Very Severe	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	water insoluble	100%	96	4	84			3.803			130.26			Very severe	Very Severe	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	water insoluble	100%	96	5	37			2.783			78.8			Severe	Very Severe	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	water insoluble	100%	n.p.	-	1.30			1.11						Severe	Severe	Casteron et al. (1996)
2,5-Dimethylhexanediol	110-03-2	solid	water insoluble	20%	99.5	1	12			0.415			18.2			Mild	Mild	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	solid	water insoluble	20%	99.5	2	10.7			0.979			25.3			Moderate	Mild	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	solid	water insoluble	20%	99.5	3	6.7			0.925			20.5			Mild	Mild	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	solid	water insoluble	20%	99.5	4	21.33			0.68			31.533			Moderate	Mild	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	solid	water insoluble	20%	99.5	5	4.7			0.245			8.3			Mild	Mild	Balls et al. (1995)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	1							10			Mild	Mild	Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	2							10			Mild	Mild	Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	3							14			Mild	Mild	Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	4							11			Mild	Mild	Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	5							11			Mild	Mild	Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	6							14			Mild	Mild	Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	7							10			Mild	Mild	Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	8							10			Mild	Mild	Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	9	6.3	6	1.7	0.204	6	0.056	9	6	1.4	Mild	Mild	Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	10							no data			n.a.	Mild	Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	11							4			Mild	Mild	Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	12							22			Mild	Mild	Gautheron et al. (1994)
Dodecane	112-40-3	liquid	n.p.	100%	n.p.	-	0.086			0.006						Mild	Mild	Casteron et al. (1996)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	1							-1			Mild	Mild	Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	2							0			Mild	Mild	Gautheron et al. (1994)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	3							-8			Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	4							2			Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	5							2			Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	6							1			Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	7							1			Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	8							-6			Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	9	0.8	6	0.5	0.01	6	0.014	1	6	0.6	Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	10							-1			Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	11							3			Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	12							1			Mild		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	1	31			2.893			74.4			Severe		Balls et al. (1995)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2	21.3			2.123			53.2			Moderate		Balls et al. (1995)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	3	16.3			3.134			63.3			Severe		Balls et al. (1995)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	4	36			4.134			98.01			Very severe		Balls et al. (1995)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	5	30			2.277			64.2			Severe		Balls et al. (1995)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	1							58			Severe		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2							67			Severe		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	3							70			Severe		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	4							45			Moderate		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	5							60			Severe		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	6							64			Severe		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	7							58			Severe		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	8							51			Moderate		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	9	22.3	6	4.1	1.56	6	0.316	46	6	6.6	Moderate		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	11							104			Severe		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	12							45			Moderate		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	1 (1)	17.6	3	2.3	1.265	3	0.252	36.6	3	6.0	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	1 (2)	16.4	3	5.5	1.415	3	0.389	37.6	3	10.8	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	1 (3)	13.7	3	1.5	1.062	3	0.322	29.6	3	6.4	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	1 (4)	12.7	3	1.0	1.933	3	0.397	41.7	3	5.8	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	1 (5)	14.7	3	2.1	1.125	3	0.162	31.5	3	4.5	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	1 (6)	12.7	3	14.9	1.995	3	0.035	42.6			Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	1 (7)	18.7	3	1.5	2.445	3	0.733	55.4			Severe		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2 (1)	13.3	3	1.0	2.626	3	0.909	52.7	3	12.8	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2 (2)	17.0	3	2.3	2.504	3	0.703	54.5	3	8.3	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2 (3)	16.3	3	4.9	3.025	3	0.699	61.7	3	7.8	Severe		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2 (4)	17.3	3	1.5	2.857	3	0.250	60.2	3	4.9	Severe		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2 (5)	14.7	3	2.1	2.636	3	0.427	54.2	3	5.0	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2 (6)	17.6	3	0.6	3.718	3	0.798	73.4			Severe		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2 (7)	15.0	3	2.6	3.267	3	0.545	64.0			Severe		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2 (8)	13.0	3	0.6	2.561	3	0.867	51.4			Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	3 (1)	16.6	3	2.1	2.027	3	1.026	47.0	3	14.3	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	3 (2)	18.0	3	2.9	1.831	3	0.061	45.4	3	2.0	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	3 (3)	19.3	3	2.6	1.673	3	0.071	44.4	3	3.0	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	3 (4)	22.0	3	2.6	1.583	3	0.426	45.7	3	8.5	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	3 (5)	18.6	3	1.5	2.395	3	0.380	54.6	3	4.5	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	3 (6)	17.0	3	1.2	1.853	3	0.268	44.8	3	5.1	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	3 (7)	19.3	3	3.8	1.527	3	0.344	42.2	3	8.8	Moderate		Southee (1998)
Ethanol (#14)	64-17-5	liquid	n.p.	100%	n.p.	-							52.7			Moderate	Moderate	Swanson and Harbell (2000)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	1							99			Severe		Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	2							100			Severe		Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	3							128			Severe		Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	4							75			Severe		Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	5							75			Severe		Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	6							85			Severe		Gautheron et al. (1994)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	7							94			Severe	Severe	Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	8							93			Severe	Severe	Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	9	61.7	6	1.9	1.515	6	0.134	84	6	1.2	Severe	Severe	Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	10							75			Severe	Severe	Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	11							101			Severe	Severe	Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	12							86			Severe	Severe	Gautheron et al. (1994)
Ethyl acetate	141-78-6	liquid	water soluble	100%	n.p.	99	8.7			0.737			19.7			Mild	Moderate	Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	water soluble	100%	n.p.	99	5.7			1.513			28.4			Moderate	Moderate	Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	water soluble	100%	n.p.	99	3	9		2.543			47.1			Moderate	Moderate	Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	water soluble	100%	n.p.	99	4	13.33		2.065			44.31			Moderate	Moderate	Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	water soluble	100%	n.p.	99	5	11		0.64			20.6			Mild	Moderate	Balls et al. (1995)
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	1							26			Moderate	Moderate	Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	2							38			Moderate	Moderate	Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	3							31			Moderate	Moderate	Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	4							33			Moderate	Moderate	Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	5							21			Moderate	Moderate	Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	6							29			Moderate	Moderate	Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	7							28			Moderate	Moderate	Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	8							38			Moderate	Moderate	Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	9	24	6	2.9	0.117	6	0.007	26	6	3.8	Moderate	Moderate	Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	10							no data			n.a.	Moderate	Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	11							38			Moderate	Moderate	Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	12							42			Moderate	Moderate	Gautheron et al. (1994)
2-Ethylhexanol	104-76-7	liquid	water soluble	100%	n.p.	-	0.321			0.352						Moderate	Moderate	Casteron et al. (1996)
2-Ethyl-1-hexanol	104-76-7	liquid	water soluble	100%	n.p.	99	1	8.3		3.58			62			Severe	Severe	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	water soluble	100%	n.p.	99	2	9		1.279			28.2			Moderate	Nonsevere	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	water soluble	100%	n.p.	99	3	4.3		1.761			30.7			Moderate	Nonsevere	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	water soluble	100%	n.p.	99	4	7		3.347			58.71			Severe	Severe	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	water soluble	100%	n.p.	99	5	7		0.837			19.6			Mild	Severe	Balls et al. (1995)
Ethylhexyl acid phosphate ester	-	liquid	moderate	100%	n.p.	-	117.3			0.880			130.5			Severe	Severe	Bailey et al. (2004)
5-Ethylidene-2-norbornene	16219-75-3	liquid	negligible	100%	n.p.	-	5.7			0.207			8.8			Mild	Mild	Bailey et al. (2004)
Ethyl-2-methylacetoacetate	609-14-3	liquid	water soluble*	100%	n.p.	97	1	26.7		0.052			27.5			Moderate	Mild	Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	water soluble*	100%	n.p.	97	2	14.3		-0.014			14.1			Mild	Mild	Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	water soluble*	100%	n.p.	97	3	5.7		-0.012			5.5			Mild	Mild	Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	water soluble*	100%	n.p.	97	4	5.33		0.014			5.543			Mild	Mild	Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	water soluble*	100%	n.p.	97	5	18.7		0.061			19.6			Mild	Mild	Balls et al. (1995)
3-Ethyltoluene	620-14-4	liquid	n.p.	100%	n.p.	-	0.029			0.009						Mild	Mild	Casteron et al. (1996)
Ethyl trimethyl acetate	3938-95-2	liquid	water insoluble*	100%	n.p.	99	1	10.3		1.136			27.4			Moderate	Mild	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	water insoluble*	100%	n.p.	99	2	5		1.916			33.7			Moderate	Mild	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	water insoluble*	100%	n.p.	99	3	1.3		0.609			10.5			Mild	Mild	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	water insoluble*	100%	n.p.	99	4	5.33		0.22			8.633			Mild	Mild	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	water insoluble*	100%	n.p.	99	5	3.6		0.357			9			Mild	Mild	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	water insoluble*	100%	n.p.	-	0.330			0.257						Moderate	Moderate	Casteron et al. (1996)
Eye Make-Up Remover (HZH)	-	n.p.	n.p.	100%	n.p.	-	0.034			0.068						Mild	Mild	Casteron et al. (1996)
Eye Make-Up Remover (HZH) 100%	-	n.p.	n.p.	10%	n.p.	-				0.02	3	0.016	0.2			Nonsevere	Nonsevere	Gettings et al. (1996)
Facial Cleansing Foam (HZR) 25%	-	n.p.	n.p.	10%	n.p.	-				0.239	3	0.02	4.1			Nonsevere	Nonsevere	Gettings et al. (1996)
Facial Cleanser (HZZ)	-	n.p.	n.p.	100%	n.p.	-	0.067			0.001						Mild	Mild	Casteron et al. (1996)
Facial Cleanser (HZZ) 100%	-	n.p.	n.p.	10%	n.p.	-				0.004	3	0.004	1.8			Nonsevere	Nonsevere	Gettings et al. (1996)
Floor Cleaner (#10)	-	liquid	n.p.	100%	n.p.	-	45.2	5		1.675	5		70.3	5		Severe	Severe	Swanson et al. (1995)
Floor Cleaner (#2)	-	liquid	n.p.	100%	n.p.	-	-2.1	5		0.119	5		-0.3	5		Nonirritant	Nonirritant	Swanson et al. (1995)
Floor Stripper (#14)	-	liquid	n.p.	100%	n.p.	-	122.5	5		2.318	5		157.3	5		Severe	Severe	Swanson et al. (1995)
Floor Stripper (#17)	-	liquid	n.p.	100%	n.p.	-	180.5	5		2.38	5		216.2	5		Severe	Severe	Swanson et al. (1995)
Floor Stripper (#18)	-	liquid	n.p.	100%	n.p.	-	407.1	5		2.481	5		444.3	5		Severe	Severe	Swanson et al. (1995)
Foam Bath (HZL)	-	n.p.	n.p.	100%	n.p.	-	0.094			0.238						Moderate	Moderate	Casteron et al. (1996)
Foam Bath (HZL) 100%	-	n.p.	n.p.	10%	n.p.	-				0.912	3	0.261	18.6			Severe	Severe	Gettings et al. (1996)
Fomesafen	72128-02-0	solid	water soluble	20%	97.5	1	2.6			2.859			45.5			Moderate	Severe	Balls et al. (1995)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Fomesafen	72128-02-0	solid	water soluble	20%	97.5	2	4.3			9.837			151.9			Very severe		Balls et al. (1995)
Fomesafen	72128-02-0	solid	water soluble	20%	97.5	3	6.3			3.904			64.9			Severe	Nonsevere	Balls et al. (1995)
Fomesafen	72128-02-0	solid	water soluble	20%	97.5	4	13			0.668			23.023			Mild		Balls et al. (1995)
Fomesafen	72128-02-0	solid	water soluble	20%	97.5	5	5.7			0.834			18.2			Mild		Balls et al. (1995)
Furan	110-00-9	liquid	n.p.	100%	n.p.	1							73			Severe		Gautheron et al. (1994)
Furan	110-00-9	liquid	n.p.	100%	n.p.	2							63			Severe		Gautheron et al. (1994)
Furan	110-00-9	liquid	n.p.	100%	n.p.	3							61			Severe		Gautheron et al. (1994)
Furan	110-00-9	liquid	n.p.	100%	n.p.	4							65			Severe		Gautheron et al. (1994)
Furan	110-00-9	liquid	n.p.	100%	n.p.	5							33			Moderate		Gautheron et al. (1994)
Furan	110-00-9	liquid	n.p.	100%	n.p.	6							34			Moderate		Gautheron et al. (1994)
Furan	110-00-9	liquid	n.p.	100%	n.p.	7							87			Severe		Gautheron et al. (1994)
Furan	110-00-9	liquid	n.p.	100%	n.p.	8							48			Moderate		Gautheron et al. (1994)
Furan	110-00-9	liquid	n.p.	100%	n.p.	9	20.6	6	2.5	1.97	6	0.197	50	6	4	Moderate		Gautheron et al. (1994)
Furan	110-00-9	liquid	n.p.	100%	n.p.	10							39			Moderate		Gautheron et al. (1994)
Furan	110-00-9	liquid	n.p.	100%	n.p.	11							68			Severe		Gautheron et al. (1994)
Furan	110-00-9	liquid	n.p.	100%	n.p.	12							51			Moderate		Gautheron et al. (1994)
Gel Cleanser (HZE)	-	n.p.	n.p.	100%	n.p.	-	0.009			0.124						Mild	Mild	Casterton et al. (1996)
Gel Cleanser (HZE) 100%	-	n.p.	n.p.	10%	n.p.	-				0.194	3	0.048	3.1			Nonsevere	Nonsevere	Gettings et al. (1996)
General Cleaner (#11)	-	liquid	n.p.	100%	n.p.	-	77.9	5		0.359	5		83.3	5		Severe	Severe	Swanson et al. (1995)
General Cleaner (#12)	-	liquid	n.p.	100%	n.p.	-	95.5	5		1.197	5		113.5	5		Severe	Severe	Swanson et al. (1995)
Glass Cleaner (#19)	-	liquid	n.p.	100%	n.p.	-	98.3	5		2.499	5		135.8	5		Severe	Severe	Swanson et al. (1995)
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	1							63			Severe		Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	2							81			Severe		Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	3							90			Severe		Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	4							62			Severe		Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	5							108			Severe		Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	6							66			Severe		Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	7							90			Severe		Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	8							57			Severe		Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	9	85.2	6	5.6	0.154	6	0.041	88	6	5.3	Severe		Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	11							75			Severe		Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	12							63			Severe		Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	1							2			Mild		Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	2							1			Mild		Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	3							1			Mild		Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	4							1			Mild		Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	5							0			Mild		Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	6							-4			Nonirritant		Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	7							1			Mild	Mild	Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	8							4			Mild		Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	9	-0.2	6	0.5	-0.005	6	0.005	0	6	0.5	Mild		Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	10							2			Mild		Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	11							0			Mild		Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	12							-1			Nonirritant		Gautheron et al. (1994)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	1	-2			-0.001			-2			Mild		Balls et al. (1995)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	2	-0.7			0.029			-0.2			Mild		Balls et al. (1995)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	3	0			0.018			0.3			Mild		Balls et al. (1995)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	4	3			0.005			3.08			Mild		Balls et al. (1995)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	5	0			0.01			0.1			Mild		Balls et al. (1995)
Glycerol	56-81-5	liquid	water soluble	100%	n.p.	-	-0.020			0.013						Mild	Mild	Casterton et al. (1996)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	1 (1)	0.6	3	0.6	-0.005	3	0.002	0.6	3	0.6	Mild		Southee (1998)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	1 (2)	0.3	3	1.0	-0.003	3	0.002	0.3	3	1.0	Mild		Southee (1998)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	2 (1)	0.6	3	0.6	0.012	3	0.007	0.8	3	0.6	Nonirritant		Southee (1998)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	2 (2)	0.7	3	0.6	0.008	3	0.009	0.8	3	0.7	Nonirritant		Southee (1998)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	3 (1)	1.0	3	0.6	-0.003	3	0.005	1.0	3	0.6	Nonirritant		Southee (1998)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	3 (2)	0.7	3	0.0	0.007	3	0.011	0.8	3	0.2	Nonirritant		Southee (1998)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	1							18			Mild		Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	2							24			Mild		Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	3							25			Mild		Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	4							14			Mild		Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	5							13			Mild		Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	6							6			Mild		Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	7							15			Mild		Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	8							18			Mild		Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	9	16.6	6	4.5	0.065	6	0.082	18	6	4.7	Mild		Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	10							4			Mild		Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	11							23			Mild		Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	12							21			Mild		Gautheron et al. (1994)
Hand Soap (HZU) 25%	-	n.p.	n.p.	10%	n.p.	-				0.293	3	0.09	5.5			Nonsevere	Nonsevere	Gettings et al. (1996)
Heavy Duty Cleaner (#15)	-	liquid	n.p.	100%	n.p.	-	323.3	5		2.24	5		357.1	5		Severe	Severe	Swanson et al. (1995)
Heavy Duty Cleaner/Degreaser (#9)	-	liquid	n.p.	100%	n.p.	-	315.4	5		2.619	5		354.7	5		Severe	Severe	Swanson et al. (1995)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	1							93			Severe		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	2							40			Moderate		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	3							53			Moderate		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	4							33			Moderate		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	5							91			Severe		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	6							42			Moderate		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	7							82			Severe		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	8							76			Severe		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	9	18.3	6	3.6	3.438	6	0.562	70	6	6.9	Severe		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	11							48			Moderate		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	12							102			Severe		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	1 (1)	13.3	3	2.0	0.654	3	0.273	23.1	3	5.9	Mild		Southee (1998)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	1 (2)	9.7	3	4.2	0.499	3	0.109	17.2	3	5.8	Mild		Southee (1998)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	2 (1)	13.7	3	3.2	1.398	3	0.601	34.6	3	12.1	Moderate		Southee (1998)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	2 (2)	13.0	3	4.4	1.743	3	0.871	39.1	3	16.4	Moderate		Southee (1998)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	3 (1)	17.3	3	1.0	0.958	3	0.100	31.7	3	2.3	Moderate		Southee (1998)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	3 (2)	17.7	3	2.1	0.818	3	0.607	29.9	3	11.2	Moderate		Southee (1998)
1,5-Hexadiene	592-42-7	liquid	n.p.	100%	n.p.	-	0.164			0.085						Mild	Mild	Casterton et al. (1996)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	1							2			Mild		Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	2							2			Mild		Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	3							2			Mild		Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	4							0			Mild		Gautheron et al. (1994)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Hexane	110-54-3	liquid	n.p.	100%	n.p.	5							2			Mild	Mild	Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	6							1			Mild	Mild	Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	7							3			Mild	Mild	Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	8							1			Mild	Mild	Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	9	1.3	6	1.8	0.002	6	0.002	1	6	1.8	Mild	Mild	Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	10							-1			Nonirritant	Nonirritant	Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	11							-2			Nonirritant	Nonirritant	Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	12							6			Mild	Mild	Gautheron et al. (1994)
n-Hexanol	111-27-3	liquid	water insoluble*	100%	98	1	17.7			3.591			71.5			Severe	Severe/Very Severe	Balls et al. (1995)
n-Hexanol	111-27-3	liquid	water insoluble*	100%	98	2	16			4.509			83.6			Very severe	Severe/Very Severe	Balls et al. (1995)
n-Hexanol	111-27-3	liquid	water insoluble*	100%	98	3	7			3.746			63.2			Severe	Severe/Very Severe	Balls et al. (1995)
n-Hexanol	111-27-3	liquid	water insoluble*	100%	98	4	15.33			2.191			48.19			Moderate	Severe/Very Severe	Balls et al. (1995)
n-Hexanol	111-27-3	liquid	water insoluble*	100%	98	5	10.7			2.145			42.9			Moderate	Severe/Very Severe	Balls et al. (1995)
Imidazole	288-32-4	solid	water soluble	20%	99	1	68.3			2.232			116.8			Very severe	Very Severe	Balls et al. (1995)
Imidazole	288-32-4	solid	water soluble	20%	99	2	93			2.724			133.9			Very severe	Very Severe	Balls et al. (1995)
Imidazole	288-32-4	solid	water soluble	20%	99	3	62.3			2.741			103.4			Very severe	Very Severe	Balls et al. (1995)
Imidazole	288-32-4	solid	water soluble	20%	99	4	97.34			1.424			118.7			Very severe	Very Severe	Balls et al. (1995)
Imidazole	288-32-4	solid	water soluble	20%	99	5	54.3			2.431			90.8			Very severe	Very Severe	Balls et al. (1995)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	1							75			Severe	Severe	Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	2							73			Severe	Severe	Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	3							140			Severe	Severe	Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	4							81			Severe	Severe	Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	5							96			Severe	Severe	Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	6							62			Severe	Severe	Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	7							82			Severe	Severe	Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	8							122			Severe	Severe	Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	9	40.3	6	9.9	1.598	6	0.271	64	6	11.2	Severe	Severe	Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	10							81			Severe	Severe	Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	11							114			Severe	Severe	Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	12							65			Severe	Severe	Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	1 (1)	91.3	3	2.1	3.379	3	0.106	142.0	3	3.0	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	1 (2)	88.0	3	7.5	3.306	3	0.597	137.6	3	6.8	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	1 (3)	73.7	3	10.1	2.565	3	1.063	112.2	3	24.7	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	1 (4)	86.0	3	9.6	3.006	3	1.078	131.1	3	6.7	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	1 (5)	97.0	3	15.5	3.241	3	0.233	145.6	3	12.0	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	1 (6)	115.3	3	9.1	3.150	3	0.181	162.6	3		Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	1 (7)	70.3	3	4.5	3.681	3	0.691	125.5	3		Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	2 (1)	85.7	3	9.8	3.490	3	0.309	138.1	3	13.0	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	2 (2)	88.0	3	13.0	3.471	3	0.381	140.1	3	11.9	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	2 (3)	86.3	3	6.0	3.240	3	0.651	134.9	3	9.4	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	2 (4)	92.3	3	7.9	4.324	3	1.048	157.2	3	12.5	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	2 (5)	88.0	3	16.7	3.308	3	0.695	137.6	3	6.8	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	2 (6)	97.3	3	12.9	3.709	3	0.866	152.9			Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	2 (7)	100.0	3	9.1	3.316	3	0.183	148.7			Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	3 (1)	83.0	3	14.8	3.774	3	0.828	139.6	3	26.0	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	3 (2)	91.7	3	9.3	3.232	3	0.702	140.1	3	18.9	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	3 (3)	80.4	3	3.1	2.907	3	0.642	124.0	3	6.9	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	3 (4)	82.3	3	2.1	3.093	3	0.635	128.7	3	8.2	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	3 (5)	76.6	3	8.3	3.118	3	0.464	123.4	3	14.8	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	3 (6)	76.3	3	8.7	2.862	3	0.292	121.2	3	4.6	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	3 (7)	77.3	3	2.0	3.602	3	0.413	131.3	3	8.2	Very severe	Very Severe	Southee (1998)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	1							0			Mild	Mild	Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	2							1			Mild	Mild	Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	3							6			Mild	Mild	Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	4							0			Mild	Mild	Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	5							4			Mild	Mild	Gautheron et al. (1994)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	6							0			Mild	Mild	Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	7							1			Mild	Mild	Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	8							12			Mild	Mild	Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	9	0.2	6	0.4	-0.001	6	0.003	0	6	0.4	Mild	Mild	Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	10							no data			n.a.	Mild	Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	11							6			Mild	Mild	Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	12							-4			Nonirritant	Mild	Gautheron et al. (1994)
Isobutanol	78-83-1	liquid	water insoluble*	100%	99.9	1	17			2.494			54.4			Moderate	Moderate	Balls et al. (1995)
Isobutanol	78-83-1	liquid	water insoluble*	100%	99.9	2	20			3.598			74			Severe	Moderate	Balls et al. (1995)
Isobutanol	78-83-1	liquid	water insoluble*	100%	99.9	3	19			3.248			67.7			Severe	Moderate	Balls et al. (1995)
Isobutanol	78-83-1	liquid	water insoluble*	100%	99.9	4	26			1.052			41.78			Moderate	Moderate	Balls et al. (1995)
Isobutanol	78-83-1	liquid	water insoluble*	100%	99.9	5	21.4			1.39			42.2			Moderate	Moderate	Balls et al. (1995)
Isobutanol	78-83-1	liquid	water insoluble*	100%	n.p.	-	0.453			0.688						Severe	Severe	Casterton et al. (1996)
Isopropanol	67-63-0	liquid	water soluble	100%	99.9	1	11.7			1.868			39.7			Moderate	Moderate	Balls et al. (1995)
Isopropanol	67-63-0	liquid	water soluble	100%	99.9	2	23.3			2.409			59.5			Severe	Moderate	Balls et al. (1995)
Isopropanol	67-63-0	liquid	water soluble	100%	99.9	3	16			3.755			72.3			Severe	Severe	Balls et al. (1995)
Isopropanol	67-63-0	liquid	water soluble	100%	99.9	4	30.66			3.189			78.5			Severe	Severe	Balls et al. (1995)
Isopropanol	67-63-0	liquid	water soluble	100%	99.9	5	18.3			1.4			39.3			Moderate	Moderate	Balls et al. (1995)
Isopropanol	67-63-0	liquid	water soluble	100%	n.p.	-	0.593			0.526						Moderate	Moderate	Casterton et al. (1996)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	1							53			Moderate	Moderate	Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	2							50			Moderate	Moderate	Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	3							48			Moderate	Moderate	Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	4							28			Moderate	Moderate	Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	5							45			Moderate	Moderate	Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	6							35			Moderate	Moderate	Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	7							48			Moderate	Moderate	Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	8							43			Moderate	Moderate	Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	9	7.8	6	0.9	3.653	6	0.496	63	6	7.3	Severe	Severe	Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	10							no data			n.a.	Severe	Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	11							89			Severe	Severe	Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	12							48			Moderate	Moderate	Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	1							81			Severe	Severe	Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	2							82			Severe	Severe	Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	3							103			Severe	Severe	Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	4							76			Severe	Severe	Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	5							92			Severe	Severe	Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	6							68			Severe	Severe	Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	7							90			Severe	Severe	Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	8							62			Severe	Severe	Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	9	16.2	6	4.3	5.742	6	1.462	102	6	24.8	Severe	Severe	Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	10							no data			n.a.	Severe	Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	11							76			Severe	Severe	Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	12							55			Moderate	Moderate	Gautheron et al. (1994)
Liquid Soap No. 2 (HZW) 25%	-	n.p.	n.p.	10%	n.p.	-				0.352	3	0.1	5.6			Nonsevere	Nonsevere	Gettings et al. (1996)
Liquid Soap No. 1 (HZB) 25%	-	n.p.	n.p.	10%	n.p.	-				0.199	3	0.024	2.3			Nonsevere	Nonsevere	Gettings et al. (1996)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	1							3			Mild	Mild	Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	2							6			Mild	Mild	Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	3							3			Mild	Mild	Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	4							3			Mild	Mild	Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	5							0			Mild	Mild	Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	6							1			Mild	Mild	Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	7							7			Mild	Mild	Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	8							3			Mild	Mild	Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	9	0.5	6	0.5	0.016	6	0.004	1	6	0.5	Mild	Mild	Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	10							no data			n.a.	Mild	Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	11							0			Mild	Mild	Gautheron et al. (1994)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	12							6			Mild		Gautheron et al. (1994)
Maneb	12427-38-2	solid	water soluble	20%	90	1	67.6			-0.045			67			Severe		Balls et al. (1995)
Maneb	12427-38-2	solid	water soluble	20%	90	2	17			-0.008			16.9			Mild	Nonsevere	Balls et al. (1995)
Maneb	12427-38-2	solid	water soluble	20%	90	3	21			-0.002			21			Mild		Balls et al. (1995)
Maneb	12427-38-2	solid	water soluble	20%	90	4	56.33			0.495			63.76			Severe		Balls et al. (1995)
Maneb	12427-38-2	solid	water soluble	20%	90	5	33.3			0.029			33.8			Moderate		Balls et al. (1995)
Meat Room Degreaser (#3)	-	liquid	n.p.	100%	n.p.	-	99.3	5		2.733	5		140.3	5		Severe	Severe	Swanson et al. (1995)
2-Mercaptopyrimidine	1450-85-7	solid	n.p.	20%	n.p.	1							0			Mild		Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	n.p.	20%	n.p.	2							-1			Nonirritant		Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	n.p.	20%	n.p.	3							-1			Nonirritant		Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	n.p.	20%	n.p.	4							1			Mild		Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	n.p.	20%	n.p.	5							0			Mild		Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	n.p.	20%	n.p.	6							1			Mild		Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	n.p.	20%	n.p.	7							0			Mild		Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	n.p.	20%	n.p.	8							-8			Nonirritant		Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	n.p.	20%	n.p.	9	-0.2	6	0.4	-0.004	6	0.002	0	6	0.4	Mild		Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	n.p.	20%	n.p.	10							0			Mild		Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	n.p.	20%	n.p.	11							-4			Nonirritant		Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	n.p.	20%	n.p.	12							-3			Nonirritant		Gautheron et al. (1994)
Metal Cleaner (#20)	-	liquid	n.p.	100%	n.p.	-	344.2	5		3.182	5		391.9	5		Severe	Severe	Swanson et al. (1995)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	1							88			Severe		Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	2							88			Severe		Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	3							54			Moderate		Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	4							71			Severe		Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	5							81			Severe		Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	6							108			Severe		Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	7							37			Moderate		Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	8							19			Mild		Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	9	73.7	6	6	1.698	6	0.56	99	6	12.8	Severe		Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	11							179			Severe		Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	12							102			Severe		Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	1							61			Severe		Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	2							69			Severe		Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	3							66			Severe		Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	4							47			Moderate		Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	5							48			Moderate		Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	6							62			Severe		Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	7							65			Severe		Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	8							62			Severe		Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	9	45.1	6	7.1	0.8	6	0.137	57	6	8.9	Severe		Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	11							74			Severe		Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	12							88			Severe		Gautheron et al. (1994)
Methyl acetate	79-20-9	liquid	water soluble	100%	98	1	51.6			1.301			71.2			Severe		Balls et al. (1995)
Methyl acetate	79-20-9	liquid	water soluble	100%	98	2	42			0.299			46.5			Moderate		Balls et al. (1995)
Methyl acetate	79-20-9	liquid	water soluble	100%	98	3	38.3			0.887			51.6			Moderate	Moderate	Balls et al. (1995)
Methyl acetate	79-20-9	liquid	water soluble	100%	98	4	43.1			0.72			53.9			Moderate		Balls et al. (1995)
Methyl acetate	79-20-9	liquid	water soluble	100%	98	5	45.3			0.384			51.1			Moderate		Balls et al. (1995)
Methyl acetate	79-20-9	liquid	water soluble	100%	n.p.	-	1.07			0.236						Moderate	Moderate	Casterton et al. (1996)
Methyl cyanoacetate	105-34-0	liquid	water soluble*	100%	99	1	16.3			0.002			16.3			Mild		Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	water soluble*	100%	99	2	6.7			-0.052			5.9			Mild		Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	water soluble*	100%	99	3	10.3			-0.015			10.1			Mild	Mild	Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	water soluble*	100%	99	4	17.33			0.013			17.53			Mild		Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	water soluble*	100%	99	5	11			-0.003			11			Mild		Balls et al. (1995)
Methyl cyclopentadiene dimer	-	liquid	negligible	100%	n.p.	-	0.7			0.001			0.7			Mild	Mild	Bailey et al. (2004)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Methylcyclopentane	96-37-7	liquid	water insoluble*	100%	>99	1	1.3			0.169			3.8			Mild		Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	water insoluble*	100%	>99	2	2.3			0.152			4.6			Mild		Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	water insoluble*	100%	>99	3	0.3			0.071			1.4			Mild	Mild	Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	water insoluble*	100%	>99	4	1			0.047			1.71			Mild		Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	water insoluble*	100%	>99	5	0.3			0.161			2.7			Mild		Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	1	68			1.665			93			Very severe		Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	2	51.3			1.069			67.4			Severe		Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	3	34			1.212			52.2			Moderate		Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	4	58			1.38			78.71			Severe		Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	5	51.7			0.607			60.8			Severe		Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	n.p.	-	1.110			0.395						Moderate	Moderate	Casterton et al. (1996)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	1 (1)	47.6	3	5.9	1.706	3	0.679	73.3	3	15.9	Severe		Southee (1998)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	1 (2)	48	3	2.1	1.32	3	0.303	67.8	3	5.7	Severe		Southee (1998)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	2 (1)	61	3	2.9	3.183	3	0.86	108.7	3	11.9	Very severe		Southee (1998)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	2 (2)	62	3	6.7	2.648	3	1.074	101.7	3	21.1	Very severe		Southee (1998)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	3 (1)	55.7	3	5.0	0.972	3	0.479	70.2	3	3.5	Severe		Southee (1998)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	3 (2)	54.4	3	1.5	1.278	3	0.359	73.5	3	6.4	Severe		Southee (1998)
Methyl isobutyl ketone	108-10-1	liquid	water insoluble*	100%	98	1	4.7			0.273			8.8			Mild		Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	water insoluble*	100%	98	2	8.7			0.759			20.1			Mild		Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	water insoluble*	100%	98	3	5.7			0.307			10.3			Mild	Mild	Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	water insoluble*	100%	98	4	8			0.35			13.25			Mild		Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	water insoluble*	100%	98	5	5.7			0.305			10.3			Mild		Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	water insoluble*	100%	n.p.	-	0.413			0.172						Moderate	Moderate	Casterton et al. (1996)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	1							22			Mild		Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	2							25			Mild		Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	3							27			Moderate		Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	4							19			Mild		Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	5							21			Mild		Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	6							23			Mild		Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	7							16			Mild		Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	8							16			Mild		Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	9	11.2	6	2.7	0.546	6	0.244	19	6	3.1	Mild		Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	11							20			Mild		Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	12							11			Mild		Gautheron et al. (1994)
1-Methylpropyl benzene	135-98-8	liquid	n.p.	100%	n.p.	-	0.041			0.005						Mild	Mild	Casterton et al. (1996)
Mild Shampoo (HZJ)	-	n.p.	n.p.	100%	n.p.	-	-0.007			0.01						Mild	Mild	Casterton et al. (1996)
Mild Shampoo (HZJ) 25%	-	n.p.	n.p.	10%	n.p.	-				0.05	3	0.025	0.1			Nonsevere	Nonsevere	Gettings et al. (1996)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	1							2			Mild		Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	2							1			Mild		Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	3							0			Mild		Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	4							1			Mild		Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	5							0			Mild		Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	6							0			Mild		Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	7							1			Mild		Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	8							-4			Nonirritant		Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	9	0.4	6	1.4	0.005	6	0.004	1	6	1.4	Mild		Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	11							-3			Nonirritant		Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	12							-1			Nonirritant		Gautheron et al. (1994)
1-Naphthalene acetic acid	86-87-3	solid	water insoluble*	20%	96	1	119.4			0.095			120.8			Very severe		Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	solid	water insoluble*	20%	96	2	65.7			0.045			66.3			Severe		Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	solid	water insoluble*	20%	96	3	41			0.065			42			Moderate		Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	solid	water insoluble*	20%	96	4	86.67			0.137			88.73			Very severe		Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	solid	water insoluble*	20%	96	5	70			0.168			72.5			Severe		Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	water soluble*	20%	95	1	73.3			4.177			136			Very severe		Balls et al. (1995)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
1-Naphthalene acetic acid, Na salt	61-31-4	solid	water soluble*	20%	95	2	83			4.124			144.9			Very severe	Very Severe	Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	water soluble*	20%	95	3	73			5.864			161			Very severe		Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	water soluble*	20%	95	4	108			3.55			161.2			Very severe		Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	water soluble*	20%	95	5	94.7			3.222			143			Very severe		Balls et al. (1995)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	1							11			Mild	Mild	Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	2							8			Mild		Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	3							9			Mild		Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	4							4			Mild		Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	5							6			Mild		Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	6							7			Mild		Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	7							6			Mild		Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	8							6			Mild		Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	9	16.5	6	1.7	0.008	6	0.018	17	6	1.9	Mild		Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	10							4			Mild		Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	11							6			Mild		Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	12							7			Mild		Gautheron et al. (1994)
n-Octanol	111-87-5	liquid	water insoluble*	100%	>99	1	11			2.159			43.4			Moderate	Moderate	Balls et al. (1995)
n-Octanol	111-87-5	liquid	water insoluble*	100%	>99	2	13			4.392			78.9			Severe		Balls et al. (1995)
n-Octanol	111-87-5	liquid	water insoluble*	100%	>99	3	10			1.984			39.8			Moderate		Balls et al. (1995)
n-Octanol	111-87-5	liquid	water insoluble*	100%	>99	4	6			0.569			14.54			Mild		Balls et al. (1995)
n-Octanol	111-87-5	liquid	water insoluble*	100%	>99	5	6			1.464			28			Moderate		Balls et al. (1995)
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	1							65			Severe		Gautheron et al. (1994)
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	2							33			Moderate		Gautheron et al. (1994)
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	3							42			Moderate		Gautheron et al. (1994)
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	4							49			Moderate		Gautheron et al. (1994)
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	5							66			Severe		Gautheron et al. (1994)
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	6							48			Moderate		Gautheron et al. (1994)
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	7							37			Moderate		Gautheron et al. (1994)
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	8							25			Mild	Gautheron et al. (1994)	
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	9	27.7	6	5	2.212	6	0.377	61	6	6.9	Severe	Gautheron et al. (1994)	
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	10							no data			n.a.	Gautheron et al. (1994)	
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	11							31			Moderate	Gautheron et al. (1994)	
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	12							64			Severe	Gautheron et al. (1994)	
Parafluoraniiline	371-40-4	liquid	water insoluble	100%	99	1	17.3			0.809			29.5			Moderate	Moderate	Balls et al. (1995)
Parafluoraniiline	371-40-4	liquid	water insoluble	100%	99	2	11.3			1.006			26.4			Moderate		Balls et al. (1995)
Parafluoraniiline	371-40-4	liquid	water insoluble	100%	99	3	18.7			1.474			40.8			Moderate		Balls et al. (1995)
Parafluoraniiline	371-40-4	liquid	water insoluble	100%	99	4	18			0.8996			31.82			Moderate		Balls et al. (1995)
Parafluoraniiline	371-40-4	liquid	water insoluble	100%	99	5	13.3			0.679			23.5			Moderate		Balls et al. (1995)
Parafluoraniiline	371-40-4	liquid	water insoluble	100%	n.p.	-	0.413			0.106						Moderate		Casterton et al. (1996)
Parafluoraniiline	371-40-4	liquid	water insoluble	100%	99	1 (1)	15.3	3	1.0	1.044	3	0.413	31	3	7.2	Moderate		Southee (1998)
Parafluoraniiline	371-40-4	liquid	water insoluble	100%	99	1 (2)	16.3	3	3.5	1.243	3	0.287	35	3	6.2	Moderate		Southee (1998)
Parafluoraniiline	371-40-4	liquid	water insoluble	100%	99	2 (1)	13.3	3	2.1	1.663	3	0.372	38.3	3	7.5	Moderate		Southee (1998)
Parafluoraniiline	371-40-4	liquid	water insoluble	100%	99	2 (2)	16.0	3	4.6	1.432	3	0.531	37.5	3	12.2	Moderate		Southee (1998)
Parafluoraniiline	371-40-4	liquid	water insoluble	100%	99	3 (1)	11.0	3	1.0	0.738	3	0.154	22.1	3	2.7	Mild		Southee (1998)
Parafluoraniiline	371-40-4	liquid	water insoluble	100%	99	3 (2)	15.4	3	1.2	0.7	3	0.151	28.9	3	3.4	Moderate		Southee (1998)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	1							61			Severe	Severe	Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	2							79			Severe		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	3							75			Severe		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	4							34			Moderate		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	5							70			Severe		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	6							46			Moderate		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	7							54			Moderate		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	8							44			Moderate		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	9	49.1	6	3.4	0.084	6	0.036	50	6	3.4	Moderate		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	10							67			Severe		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	11							62			Severe		Gautheron et al. (1994)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	12							76			Severe		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	1							8			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	2							13			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	3							11			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	4							1			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	5							2			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	6							5			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	7							7			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	8							0			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	9	1.4	6	1.9	0.015	6	0.011	2	6	1.9	Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	10							3			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	11							5			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	12							9			Mild		Gautheron et al. (1994)
Petroleum wax	-	solid	negligible	100%	n.p.	-	0.3			-0.001			0.3			Mild	Mild	Bailey et al. (2004)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	1							0			Mild		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	2							1			Mild		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	3							1			Mild		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	4							0			Mild		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	5							0			Mild		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	6							1			Mild		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	7							0			Mild		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	8							-6			Nonirritant		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	9	0.7	6	0.4	-0.008	6	0.008	1	6	0.4	Mild		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	10							1			Mild		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	11							-3			Nonirritant		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	12							2			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	1							7			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	2							12			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	3							15			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	4							9			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	5							28			Moderate		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	6							6			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	7							6			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	8							16			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	9	11.1	6	1	0.143	6	0.052	13	6	1.6	Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	10							15			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	11							13			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	12							15			Mild		Gautheron et al. (1994)
Polishing Scrub (HZT)	-	n.p.	n.p.	100%	n.p.	-	0.027			0.015						Mild	Mild	Casterton et al. (1996)
Polishing Scrub (HZT) 100%	-	n.p.	n.p.	10%	n.p.	-				-0.001	3	0.001	3.7			Nonsevere	Nonsevere	Gettings et al. (1996)
Polyalkenylsuccinate ester/amine salt	-	liquid	moderate	100%	n.p.	-	2.3			0.000			2.3			Mild	Mild	Bailey et al. (2004)
Polyethylene glycol 400	25322-68-3	liquid	surfactant	100%	n.p.	1	0.3			0.019			0.6			Mild		Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	surfactant	100%	n.p.	2	2			0.036			2.5			Mild		Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	surfactant	100%	n.p.	3	-1.7			0.021			-1.3			Nonirritant	Mild	Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	surfactant	100%	n.p.	4	1			0.005			1.08			Mild		Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	surfactant	100%	n.p.	5	2.7			0.01			2.8			Mild		Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	surfactant	100%	n.p.	-	-0.015			0.008						Mild	Mild	Casterton et al. (1996)
Polyethylene glycol 600	-	liquid	surfactant	100%	n.p.	-	-0.013			0.008						Mild	Mild	Casterton et al. (1996)
Pot and Pan Cleaner (#8)	-	liquid	n.p.	100%	n.p.	-	-1.8	5		0.078	5		-0.6	5		Nonirritant	Nonirritant	Swanson et al. (1995)
Potassium cyanate	590-28-3	solid	water soluble	20%	97	1	8.7			0.499			16.2			Mild		Balls et al. (1995)
Potassium cyanate	590-28-3	solid	water soluble	20%	97	2	11			0.793			22.9			Mild		Balls et al. (1995)
Potassium cyanate	590-28-3	solid	water soluble	20%	97	3	8.3			0.248			12			Mild	Mild	Balls et al. (1995)
Potassium cyanate	590-28-3	solid	water soluble	20%	97	4	7			0.692			17.38			Mild		Balls et al. (1995)
Potassium cyanate	590-28-3	solid	water soluble	20%	97	5	3			0.234			6.5			Mild		Balls et al. (1995)
Process oil	-	liquid	negligible	100%	n.p.	-	2.7			0.004			2.7			Mild	Mild	Bailey et al. (2004)
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	98	1	120.7			-0.022			120.3			Very severe		Balls et al. (1995)

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Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	98	2	87.7			-0.234			84.2			Very severe	Very Severe	Balls et al. (1995)	
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	98	3	125			0.044			125.7			Very severe		Balls et al. (1995)	
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	98	4	121.33			0.051			123.09			Very severe		Balls et al. (1995)	
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	98	5	153.7			0.011			153.8			Very severe		Balls et al. (1995)	
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	1							117			Severe		Gautheron et al. (1994)	
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	2							156			Severe		Gautheron et al. (1994)	
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	3							109			Severe		Gautheron et al. (1994)	
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	4							111			Severe		Gautheron et al. (1994)	
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	5							164			Severe		Gautheron et al. (1994)	
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	6							174			Severe		Gautheron et al. (1994)	
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	7							103			Severe		Gautheron et al. (1994)	
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	8							50			Moderate		Gautheron et al. (1994)	
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	9	134.9	6	9.7	0.287	6	0.216	139	6	10.2	Severe	Gautheron et al. (1994)		
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	10							no data			n.a.	Gautheron et al. (1994)		
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	11							94			Severe	Gautheron et al. (1994)		
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	12							19			Mild	Gautheron et al. (1994)		
Propylene glycol	57-55-6	liquid	n.p.	100%	n.p.	-	0.076			0.024						Mild	Mild	Casterton et al. (1996)	
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	1							7			Mild		Gautheron et al. (1994)	
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	2							7			Mild	Gautheron et al. (1994)		
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	3							14			Mild	Gautheron et al. (1994)		
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	4							4			Mild	Gautheron et al. (1994)		
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	5							6			Mild	Gautheron et al. (1994)		
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	6							9			Mild	Gautheron et al. (1994)		
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	7							6			Mild	Gautheron et al. (1994)		
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	8							11			Mild	Gautheron et al. (1994)		
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	9	5.2	6	1.7	0.066	6	0.059	6	6	1.5	Mild	Mild	Gautheron et al. (1994)	
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	10							no data			n.a.		Gautheron et al. (1994)	
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	11							12			Mild		Gautheron et al. (1994)	
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	12							5			Mild		Gautheron et al. (1994)	
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	100	1 (1)	10.7	3	2.6	0.034	3	0.044	11.2	3	3.2	Mild		Southee (1998)	
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	100	1 (2)	7.0	3	0.6	0.023	3	0.026	7.4	3	0.6	Mild		Southee (1998)	
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	100	2 (1)	5.0	3	1.7	0.013	3	0.012	5.2	3	1.9	Mild		Southee (1998)	
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	100	2 (2)	3.4	3	1.5	0.016	3	0.015	3.6	3	1.6	Mild		Southee (1998)	
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	100	3 (1)	7.3	3	4.4	0.028	3	0.014	7.7	3	4.2	Mild		Southee (1998)	
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	100	3 (2)	5.6	3	0.6	0.04	3	0.051	6.2	3	0.7	Mild		Southee (1998)	
Pyridine	110-86-1	liquid	water soluble	100%	>99.9	1	73.7			4.468			140.7			Very severe		Very Severe	Balls et al. (1995)
Pyridine	110-86-1	liquid	water soluble	100%	>99.9	2	83.7			4.117			145.4			Very severe			Balls et al. (1995)
Pyridine	110-86-1	liquid	water soluble	100%	>99.9	3	61			4.763			132.4			Very severe	Balls et al. (1995)		
Pyridine	110-86-1	liquid	water soluble	100%	>99.9	4	87.33			7.445			199.02			Very severe	Balls et al. (1995)		
Pyridine	110-86-1	liquid	water soluble	100%	>99.9	5	74.7			3.204			122.7			Very severe	Balls et al. (1995)		
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	1							102			Severe	Gautheron et al. (1994)		
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	2							123			Severe	Gautheron et al. (1994)		
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	3							186			Severe	Gautheron et al. (1994)		
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	4							79			Severe	Gautheron et al. (1994)		
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	5							102			Severe	Gautheron et al. (1994)		
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	6							77			Severe	Gautheron et al. (1994)		
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	7							124			Severe	Gautheron et al. (1994)		
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	8							132			Severe	Gautheron et al. (1994)		
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	9	44.4	6	3.3	4.015	6	0.849	105	6	15.7	Severe	Gautheron et al. (1994)		
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	10							no data			n.a.	Gautheron et al. (1994)		
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	11							96			Severe	Gautheron et al. (1994)		
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	12							115			Severe	Gautheron et al. (1994)		
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	1	1			-0.047			0.3			Mild	Mild	Balls et al. (1995)	
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	2	0.3			0.002			0.4			Mild		Balls et al. (1995)	
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	3	1.7			0.028			2.1			Mild		Balls et al. (1995)	
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	4	2.34			-0.033			1.85			Mild		Balls et al. (1995)	

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	5	2			0.07			3.1			Mild		Balls et al. (1995)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	1							17			Mild		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	2							29			Moderate		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	3							8			Mild		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	4							46			Moderate		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	5							52			Moderate		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	6							24			Mild		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	7							15			Moderate		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	8							18			Moderate		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	9	57	6	5.4	0.063	6	0.04	58	6	5.8	Moderate		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	11							3			Mild		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	12							72			Severe		Gautheron et al. (1994)
Shampoo No. 1 (HZC) 25%	-	n.p.	n.p.	10%	n.p.	-				0.957	3	0.306	30.0			Severe	Severe	Gettings et al. (1996)
Shampoo No. 2 (HZX)	-	n.p.	n.p.	100%	n.p.	-	0.087			0.184						Moderate	Moderate	Casterton et al. (1996)
Shampoo No. 2 (HZX)	-	n.p.	n.p.	10%	n.p.	-				0.705	3	0.289	14.0			Severe	Severe	Gettings et al. (1996)
Shampoo No. 3 (HZM) 25%	-	n.p.	n.p.	10%	n.p.	-				0.214	3	0.049	4.3			Nonsevere	Nonsevere	Gettings et al. (1996)
Shampoo No. 4 (HZV) 25%	-	n.p.	n.p.	10%	n.p.	-				0.268	3	0.045	8.4			Nonsevere	Nonsevere	Gettings et al. (1996)
Shampoo No. 5 (HZD) 25%	-	n.p.	n.p.	10%	n.p.	-				0.241	3	0.08	2.7			Nonsevere	Nonsevere	Gettings et al. (1996)
Shampoo No. 6 (HZN) 25%	-	n.p.	n.p.	10%	n.p.	-				0.267	3	0.076	4.5			Nonsevere	Nonsevere	Gettings et al. (1996)
Shampoo No. 7 (HZA)	-	n.p.	n.p.	100%	n.p.	-	0.113			0.205						Moderate	Moderate	Casterton et al. (1996)
Shampoo No. 7 (HZA) 100%	-	n.p.	n.p.	10%	n.p.	-				0.406	3	0.156	6.6			Nonsevere	Nonsevere	Gettings et al. (1996)
Shampoo No. 8 (HZG) 25%	-	n.p.	n.p.	10%	n.p.	-				0.197	3	0.058	2.7			Nonsevere	Nonsevere	Gettings et al. (1996)
Shower Gel (HZS)	-	n.p.	n.p.	100%	n.p.	-	0.189			0.303						Moderate	Moderate	Casterton et al. (1996)
Shower Gel (HZS) 100%	-	n.p.	n.p.	10%	n.p.	-				1.548	3	0.093	35.9			Severe	Severe	Gettings et al. (1996)
Skin Cleanser (HZI)	-	n.p.	n.p.	100%	n.p.	-	0.127			0.261						Moderate	Moderate	Casterton et al. (1996)
Skin Cleanser (HZI) 100%	-	n.p.	n.p.	10%	n.p.	-				0.769	3	0.036	15.8			Severe	Severe	Gettings et al. (1996)
Sodium hydroxide (1%)	1310-73-2	liquid	water soluble	1%	reagent grade	1	100.3			4.471			167.4			Very severe		Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	liquid	water soluble	1%	reagent grade	2	80.7			3.504			133.2			Very severe		Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	liquid	water soluble	1%	reagent grade	3	88.7			3.856			146.5			Very severe	Very Severe	Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	liquid	water soluble	1%	reagent grade	4	116.66			3.628			171.08			Very severe		Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	liquid	water soluble	1%	reagent grade	5	88			2.888			132.3			Very severe		Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	liquid	water soluble	1%	n.p.	-	1.69			1.28						Severe	Severe	Casterton et al. (1996)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	reagent grade	1	232.3			3.53			285.2			Very severe		Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	reagent grade	2	173.3			3.382			224.1			Very severe		Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	reagent grade	3	197			3.849			254.7			Very severe	Very Severe	Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	reagent grade	4	283			4.329			348.27			Very severe		Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	reagent grade	5	197.3			3.321			247.2			Very severe		Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	n.p.	-	1.97			1.23						Severe	Severe	Casterton et al. (1996)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	n.p.	1 (1)	176.7	3	31.4	4.551	3	1.019	245.0	3	28.7	Very severe		Southee (1998)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	n.p.	1 (2)	172.0	3	1.7	3.676	3	0.201	227.1	3	3.4	Very severe		Southee (1998)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	n.p.	2 (1)	170.0	3	20.7	4.755	3	0.586	241.3	3	11.9	Very severe		Southee (1998)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	n.p.	2 (2)	166.7	3	12.6	4.590	3	0.405	235.5	3	7.3	Very severe		Southee (1998)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	n.p.	3 (1)	124.0	3	13.7	4.604	3	0.380	193.1	3	19.0	Very severe		Southee (1998)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	n.p.	3 (2)	165.3	3	21.2	3.303	3	0.388	214.9	3	15.5	Very severe		Southee (1998)
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	15%	98	1	4			2.884			47.3			Moderate		Balls et al. (1995)
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	15%	98	2	6			5.801			93			Very severe		Balls et al. (1995)
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	15%	98	3	3.3			3.988			63.2			Severe	Severe	Balls et al. (1995)
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	15%	98	4	1.66			3.862			59.61			Severe		Balls et al. (1995)
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	15%	98	5	7.7			3.042			53.3			Moderate		Balls et al. (1995)
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	15%	n.p.	-	0.163			0.424						Moderate	Moderate	Casterton et al. (1996)
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	10%	98	1 (1)	-0.8	3	0.0	0.408	3	0.024	5.4	3	0.4	Mild		Southee (1998)
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	10%	98	1 (2)	0.0	3	0.6	0.348	3	0.182	5.2	3	2.7	Mild		Southee (1998)
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	10%	98	2 (1)	0.7	3	1.0	1.012	3	0.461	15.9	3	7.6	Mild	Mild	Southee (1998)
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	10%	98	2 (2)	1.0	3	0.6	1.086	3	0.083	17.3	3	1.7	Mild	Mild	Southee (1998)
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	10%	98	3 (1)	0.7	3	0.6	0.518	3	0.11	8.7	3	1.4	Mild	Mild	Southee (1998)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	10%	98	3 (2)	1.3	3	0.6	0.283	3	0.064	5.6	3	1.5	Mild	Moderate	Southee (1998)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	surfactant	3%	98	1	12.3			1.29			31.7			Moderate	Moderate	Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	surfactant	3%	98	2	3.3			1.892			31.7			Moderate	Moderate	Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	surfactant	3%	98	3	0.3			1.801			27.3			Moderate	Moderate	Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	surfactant	3%	98	4	6			1.348			26.22			Moderate	Moderate	Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	surfactant	3%	98	5	0			0.82			12.3			Mild	Moderate	Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	surfactant	3%	n.p.	-	0.040			0.113						Mild	Mild	Casterton et al. (1996)
Sodium lauryl sulfate (30 %)	151-21-3	liquid	surfactant	30%	n.p.	-	0.095			0.312						Moderate	Moderate	Casterton et al. (1996)
Sodium oxalate	62-76-0	solid	water soluble	20%	>99	1	1.3			0.054			2.1			Mild	Mild	Balls et al. (1995)
Sodium oxalate	62-76-0	solid	water soluble	20%	>99	2	6.7			0.059			7.6			Mild	Mild	Balls et al. (1995)
Sodium oxalate	62-76-0	solid	water soluble	20%	>99	3	3			0.187			5.8			Mild	Mild	Balls et al. (1995)
Sodium oxalate	62-76-0	solid	water soluble	20%	>99	4	43			0.556			49.59			Moderate	Moderate	Balls et al. (1995)
Sodium oxalate	62-76-0	solid	water soluble	20%	>99	5	4			0.081			4.9			Mild	Moderate	Balls et al. (1995)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	1							2			Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	2							2			Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	3							9			Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	4							5			Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	5							3			Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	6							2			Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	7							4			Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	8							3			Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	9	1.7	6	0.9	0.103	6	0.042	3	6	1.3	Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	10							9			Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	11							11			Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	12							4			Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	99	1 (1)	8.4	3	1.2	0.128	3	0.16	10.3	3	1.4	Mild	Mild	Southee (1998)
Sodium oxalate	62-76-0	solid	water soluble	20%	99	1 (2)	3.4	3	0.6	0.071	3	0.03	4.4	3	1.0	Mild	Mild	Southee (1998)
Sodium oxalate	62-76-0	solid	water soluble	20%	99	2 (1)	-1.0	3	1.7	0.05	3	0.054	-0.3	3	1.5	Nonirritant	Nonirritant	Southee (1998)
Sodium oxalate	62-76-0	solid	water soluble	20%	99	2 (2)	-1.0	3	2.1	0.055	3	0.012	-0.1	3	2.1	Nonirritant	Nonirritant	Southee (1998)
Sodium oxalate	62-76-0	solid	water soluble	20%	99	3 (1)	2.0	3	0.6	0.051	3	0.032	2.7	3	0.9	Nonirritant	Nonirritant	Southee (1998)
Sodium oxalate	62-76-0	solid	water soluble	20%	99	3 (2)	2.3	3	1.0	0.15	3	0.022	4.5	3	1.3	Mild	Mild	Southee (1998)
Sodium perborate	10486-00-7	solid	water soluble	20%	98.6	1	10			8.908			143.6			Very severe	Very severe	Balls et al. (1995)
Sodium perborate	10486-00-7	solid	water soluble	20%	98.6	2	13.7			6.982			118.4			Very severe	Very severe	Balls et al. (1995)
Sodium perborate	10486-00-7	solid	water soluble	20%	98.6	3	10			5.749			96.2			Very severe	Very severe	Balls et al. (1995)
Sodium perborate	10486-00-7	solid	water soluble	20%	98.6	4	11			3.568			64.531			Severe	Severe	Balls et al. (1995)
Sodium perborate	10486-00-7	solid	water soluble	20%	98.6	5	9.7			3.547			62.9			Severe	Severe	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	water insoluble*	20%	97	1	24			-0.023			23.6			Mild	Mild	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	water insoluble*	20%	97	2	8.3			-0.027			7.9			Mild	Mild	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	water insoluble*	20%	97	3	14.3			-0.008			14.2			Mild	Mild	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	water insoluble*	20%	97	4	21.33			-0.045			20.65			Mild	Mild	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	water insoluble*	20%	97	5	6			0.19			8.9			Mild	Mild	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	1							5			Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	2							1			Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	3							2			Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	4							6			Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	5							0			Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	6							4			Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	7							2			Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	8							19			Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	9	2.6	6	1.4	-0.003	6	0.006	3	6	1.4	Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	10							no data			n.a.	n.a.	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	11							18			Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	12							6			Mild	Mild	Gautheron et al. (1994)
Thiadiazole alkyl derivative	-	liquid	negligible	100%	n.p.	-	7.3			0.237			10.9			Moderate	Moderate	Bailey et al. (2004)
Thiourea	62-56-6	solid	water soluble	20%	>99	1	88			4.095			149.4			Very severe	Very severe	Balls et al. (1995)
Thiourea	62-56-6	solid	water soluble	20%	>99	2	106.3			2.19			139.2			Very severe	Very severe	Balls et al. (1995)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Thiourea	62-56-6	solid	water soluble	20%	>99	3	82			3.572			135.6			Very severe	Very Severe	Balls et al. (1995)
Thiourea	62-56-6	solid	water soluble	20%	>99	4	81.01			3.76			137.44			Very severe		Balls et al. (1995)
Thiourea	62-56-6	solid	water soluble	20%	>99	5	74			1.671			99.1			Very severe		Balls et al. (1995)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	1							146			Severe	Severe	Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	2							175			Severe		Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	3							169			Severe		Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	4							152			Severe		Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	5							140			Severe		Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	6							120			Severe		Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	7							129			Severe		Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	8							173			Severe		Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	9	85.8	6	9.2	4.373	6	1.028	151	6	20.7	Severe		Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	11							203			Severe		Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	12							104			Severe		Gautheron et al. (1994)
Toilet Bowl Cleaner (#1)	-	liquid	n.p.	100%	n.p.	-	8.700	5		0.323	5		13.5	5		Mild	Mild	Swanson et al. (1995)
Toilet Bowl Cleaner (#4)	-	liquid	n.p.	100%	n.p.	-	10.5	5		0.303	5		15	5		Mild		Swanson et al. (1995)
Toluene	108-88-3	liquid	water insoluble*	100%	99	1	9.3			2.26			43.3			Moderate	Moderate	Balls et al. (1995)
Toluene	108-88-3	liquid	water insoluble*	100%	99	2	6			1.813			33.2			Moderate		Balls et al. (1995)
Toluene	108-88-3	liquid	water insoluble*	100%	99	3	5.3			2.122			37.2			Moderate		Balls et al. (1995)
Toluene	108-88-3	liquid	water insoluble*	100%	99	4	2			2.427			38.41			Moderate		Balls et al. (1995)
Toluene	108-88-3	liquid	water insoluble*	100%	99	5	4			1.473			26.1			Moderate		Balls et al. (1995)
Toluene	108-88-3	liquid	water insoluble*	100%	n.p.	-	0.420			0.805						Severe		Casterton et al. (1996)
Trichloroacetic acid (3%)	76-03-9	liquid	water soluble	3%	reagent grade	1	79.3			0.173			81.9			Very severe	Severe/Very Severe	Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	water soluble	3%	reagent grade	2	49			0.053			49.8			Moderate		Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	water soluble	3%	reagent grade	3	73.7			0.111			75.3			Severe		Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	water soluble	3%	reagent grade	4	92.33			0.042			92.97			Very severe		Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	water soluble	3%	reagent grade	5	78.4			0.067			79.3			Severe		Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	water soluble	3%	n.p.	-	0.029			0.011						Mild		Casterton et al. (1996)
Trichloroacetic acid (30%)	76-03-9	liquid	water soluble	30%	reagent grade	1	228			2.93			272			Very severe	Very Severe	Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	water soluble	30%	reagent grade	2	154.7			4.687			225			Very severe		Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	water soluble	30%	reagent grade	3	245.3			3.44			296.9			Very severe		Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	water soluble	30%	reagent grade	4	277			3.072			323.08			Very severe		Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	water soluble	30%	reagent grade	5	157			3.115			203.7			Very severe		Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	water soluble	30%	n.p.	-	1.43			0.031						Severe		Casterton et al. (1996)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	1							47			Moderate	Moderate	Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	2							42			Moderate		Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	3							78			Severe		Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	4							28			Moderate		Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	5							42			Moderate		Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	6							47			Moderate		Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	7							48			Moderate		Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	8							24			Mild		Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	9	7.7	6	1.9	5.561	6	1.398	91	6	20	Severe		Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	11							28			Moderate		Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	12							47			Moderate		Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	1							2			Mild	Mild	Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	2							4			Mild		Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	3							0			Mild		Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	4							0			Mild		Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	5							-1			Nonirritant		Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	6							1			Mild		Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	7							1			Mild		Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	8							3			Mild		Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	9	2.6	6	0.9	0.025	6	0.011	3	6	1	Mild		Gautheron et al. (1994)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	11							5			Mild		Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	12							6			Mild		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	1							25			Mild		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	2							14			Mild		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	3							26			Moderate		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	4							11			Mild		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	5							27			Moderate		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	6							7			Mild		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	7							9			Mild		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	8							15			Mild		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	9	12.5	6	1.5	0.579	6	0.369	21	6	4.5	Mild		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	10							10			Mild		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	11							7			Mild		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	12							21			Mild		Gautheron et al. (1994)
Triton X-100 (1%)	9002-93-1	liquid	surfactant	1%	n.p.	-	0.083			0.063						Mild		Casterton et al. (1996)
Triton X-100 (10%)	9002-93-1	liquid	surfactant	10%	98	1	6			5.312			85.7			Very severe		Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	surfactant	10%	98	2	6.7			4.624			76			Severe		Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	surfactant	10%	98	3	6			5.337			86.1			Very severe		Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	surfactant	10%	98	4	3.33			3.617			57.58			Severe		Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	surfactant	10%	98	5	7.7			2.567			46.2			Moderate		Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	surfactant	10%	n.p.	-	0.281			1.003						Severe		Casterton et al. (1996)
Triton X-100 (5%)	9002-93-1	liquid	surfactant	5%	98	1	5.3			4.6			74.3			Severe		Balls et al. (1995)
Triton X-100 (5%)	9002-93-1	liquid	surfactant	5%	98	2	8.3			6.553			106.6			Very severe		Balls et al. (1995)
Triton X-100 (5%)	9002-93-1	liquid	surfactant	5%	98	3	3.7			5.099			80.2			Very severe		Balls et al. (1995)
Triton X-100 (5%)	9002-93-1	liquid	surfactant	5%	98	4	5			4.79			76.79			Very severe		Balls et al. (1995)
Triton X-100 (5%)	9002-93-1	liquid	surfactant	5%	98	5	7.7			3.06			53.6			Moderate		Balls et al. (1995)
Triton X-100 (5%)	9002-93-1	liquid	surfactant	5%	n.p.	-	0.281			0.564						Moderate		Casterton et al. (1996)
Triton X-100 (5%)	9002-93-1	liquid	surfactant	10%	98	1 (1)	3.3	3	1.0	0.023	3	0.004	3.7	3	1.1	Mild		Southee (1998)
Triton X-100 (5%)	9002-93-1	liquid	surfactant	10%	98	1 (2)	1.3	3	1.0	0.035	3	0.006	1.8	3	1.0	Mild		Southee (1998)
Triton X-100 (5%)	9002-93-1	liquid	surfactant	10%	98	2 (1)	1.4	3	0.6	0.298	3	0.123	5.8	3	2.4	Mild		Southee (1998)
Triton X-100 (5%)	9002-93-1	liquid	surfactant	10%	98	2 (2)	0.0	3	0.6	0.226	3	0.086	3.4	3	1.0	Mild		Southee (1998)
Triton X-100 (5%)	9002-93-1	liquid	surfactant	10%	98	3 (1)	2.7	3	1.0	0.023	3	0.009	3.0	3	1.1	Nonirritant		Southee (1998)
Triton X-100 (5%)	9002-93-1	liquid	surfactant	10%	98	3 (2)	1.4	3	0.6	0.038	3	0.013	1.9	3	0.6	Nonirritant		Southee (1998)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	1							-1			Nonirritant		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	2							1			Mild		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	3							-1			Nonirritant		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	4							0			Mild		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	5							2			Mild		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	6							2			Mild		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	7							0			Mild		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	8							2			Mild		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	9	3	6	1.6	0.008	6	0.014	3	6	1.7	Mild		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	11							-2			Nonirritant		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	12							0			Mild		Gautheron et al. (1994)
Tween 20	9005-64-5	liquid	surfactant	n.p.	98	1	-0.7			0.006			-0.6			Mild		Balls et al. (1995)
Tween 20	9005-64-5	liquid	surfactant	n.p.	98	2	-0.3			-0.052			-1.1			Mild		Balls et al. (1995)
Tween 20	9005-64-5	liquid	surfactant	n.p.	98	3	-2			0.026			-1.6			Mild		Balls et al. (1995)
Tween 20	9005-64-5	liquid	surfactant	n.p.	98	4	2.67			0.0003			2.711			Mild		Balls et al. (1995)
Tween 20	9005-64-5	liquid	surfactant	n.p.	98	5	0.1			0.026			0.4			Mild		Balls et al. (1995)
Tween 20	9005-64-5	liquid	surfactant	100%	98	1 (1)	0.3	3	0.0	0.003	3	0.012	0.3	3	0.2	Mild		Southee (1998)
Tween 20	9005-64-5	liquid	surfactant	100%	98	1 (2)	0.0	3	1.5	0.004	3	0.01	0.0	3	1.6	Mild		Southee (1998)
Tween 20	9005-64-5	liquid	surfactant	100%	98	2 (1)	0.4	3	0.6	0.001	3	0.002	0.4	3	0.6	Mild		Southee (1998)
Tween 20	9005-64-5	liquid	surfactant	100%	98	2 (2)	0.4	3	0.6	0.003	3	0.008	0.4	3	0.5	Nonirritant		Southee (1998)
Tween 20	9005-64-5	liquid	surfactant	100%	98	3 (1)	0.0	3	0.0	0.022	3	0.018	0.3	3	0.3	Nonirritant		Southee (1998)

***In Vitro* Data for Substances Tested in the BCOP Assay: Sorted by Substance Name**

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₄₉₀	n	SD - OD ₄₉₀	<i>In Vitro</i> Score ¹	n	SD - Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	Reference
Tween 20	9005-64-5	liquid	surfactant	100%	98	3 (2)	0.0	3	1.0	0.001	3	0.022	0.0	3	1.3	Nonirritant		Southee (1998)
Tween 20	9005-64-5	liquid	surfactant	100%	n.p.	-	-0.006			0.005						Mild	Mild	Casterton et al. (1996)
Xylene	1330-20-7	liquid	n.p.	100%	n.p.	-	0.220			0.257						Moderate	Moderate	Casterton et al. (1996)

Abbreviations: CASRN=Chemical Abstract Services Registry Number; n=number of replicates; n.s.=not applicable; n.p.=not provided; OD=optical density; SD=standard deviation

¹*In Vitro* Score = mean opacity score + (15 x mean OD₄₉₀ value) represents the BCOP ocular irritancy classification assigned for each chemical in the study for each test for a specific substance

²*In Vitro* Classification represents the BCOP ocular irritancy classification assigned for each independent test result, according to the classification system used

³Consensus call represents the overall BCOP ocular irritancy classification assigned for each chemical in the study based on the majority of ocular irritancy classification calls. When there was an even number of different irritancy classifications for a test substance, the more severe irritancy classification was used for the overall classification for that test substance.

*solubility uncertain