

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

Substance	CASRN	Concentration Tested	<i>In Vivo</i> Classification (GHS)	<i>In Vivo</i> Classification (EPA)	<i>In Vivo</i> Classification (EU)	<i>In Vitro</i> Classification	Reference
Acetaldehyde	75-07-0	100%	-	-	Review Data	Severe irritant	CEC (1991)
Acetic acid	64-19-7	10%	-	-	R41	Severe Irritant	CEC (1991)
Acetone	67-64-1	100%	Category 2A	Category II	R36	Severe Irritant	Balls et al. (1995)
Acetone (F33)	67-64-1	100%	Category 2A	Category II	R36	Severe Irritant	Guerrero et al. (2004)
2-(Acetyloxy)-1-phenylethanone (F27)	-	100%	Nonirritant	Category III	Nonirritant	Nonsevere Irritant	Guerrero et al. (2004)
Allyl alcohol (F34)	107-18-6	100%	NT	NT	NT	Severe Irritant	Guerrero et al. (2004)
gamma-(Aminocarbonyl)-N-methyl-N,N-bis(1-methylethyl)-gamma-phenyl-, iodide (F14)	-	100%	Category 2A	Category II	R36	Nonsevere Irritant	Guerrero et al. (2004)
1-(5-Amino-2-methoxyphenyl) piperazine hydrochloride (F20)	-	100%	Nonirritant	Category III	Nonirritant	Severe Irritant	Guerrero et al. (2004)
tetra-Aminopyrimidine sulfate	5392-28-9	100%	Nonirritant	Category III	Nonirritant	Nonsevere Irritant	Balls et al. (1995)
Ammonium nitrate	6484-52-2	100%	Category 2B	Category III	R36	Nonsevere Irritant	Balls et al. (1995)
Ammonium nitrate (F36)	6484-52-2	100%	Category 2B	Category III	R36	Nonsevere Irritant	Guerrero et al. (2004)
L-Aspartic acid	70-47-3	100%	SCNM	SCNM	Review Data	Nonsevere Irritant	Balls et al. (1995)
Benzalkonium chloride	8001-54-5	100%	-	-	R41	Severe Irritant	CEC (1991)
Benzalkonium chloride (1 %)	8001-54-5	1%	Category 1	Category I	R41	Severe Irritant	Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	10%	Category 1	Category I	R41	Severe Irritant	Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	5%	Category 1	Category I	R41	Severe Irritant	Balls et al. (1995)
3-((Benzylthio)methyl)-6-chloro-,1,1-dioxide (F29)	-	100%	Nonirritant	Category IV	Nonirritant	Nonsevere Irritant	Guerrero et al. (2004)
Brij 35	9002-92-0	100%	-	-	nonirritant	Nonsevere Irritant	CEC (1991)
Butanol	71-36-3	100%	-	-	nonirritant	Severe Irritant	CEC (1991)
iso-Butanol	78-83-1	100%	Category 2A	Category II	R36	Severe Irritant	Balls et al. (1995)
n-Butanol (F35)	71-36-3	100%	Category 2A	Category II	R36	Severe Irritant	Guerrero et al. (2004)
2-Butoxyethyl acetate	112-07-2	100%	-	-	nonirritant	Nonsevere Irritant	CEC (1991)
N-Butyl acetate	123-86-4	100%	Nonirritant	Category III	Nonirritant	Nonsevere Irritant	Balls et al. (1995)
n-Butyl acetate (F39)	123-86-4	100%	Nonirritant	Category III	Nonirritant	Severe Irritant	Guerrero et al. (2004)
g-Butyrolactone	96-48-0	100%	Category 2A	Category II	R36	Severe Irritant	Balls et al. (1995)

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Captan 90 concentrate	133-06-2	100%	Category 1	Category I	R41	Nonsevere Irritant	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	100%	Category 2A	Category II	R36	Nonsevere Irritant	Balls et al. (1995)
Cetylpyridium bromide (F37)	140-72-7	100%	Category 1	Category I	R41	Severe Irritant	Guerriero et al. (2004)
Cetylpyridinium bromide (0.1%)	140-72-7	0.1%	Nonirritant	Category III	Nonirritant	Severe Irritant	Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	10%	Category 1	Category I	R41	Severe Irritant	Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	6%	Category 1	SCNM	R41	Severe Irritant	Balls et al. (1995)
5-Chloro-2,4-disulfamoyl chloroacetanilide (F22)	-	100%	Nonirritant	Category IV	Nonirritant	Nonsevere Irritant	Guerriero et al. (2004)
Chloroform	67-66-3	100%	-	-	Review Data	Nonsevere irritant	CEC (1991)
5-Chloro-3-methylbenzo[b]thiophene-2-sulfonyl chloride (F18)	-	100%	Nonirritant	Category III	Nonirritant	Nonsevere Irritant	Guerriero et al. (2004)
5-Chloro-N-[4-methoxy-3-(1-piperazinyl)phenyl]-3-methylbenzo[B]thiophene-2-sulfonamide monohydrochloride (F4)	-	100%	Category 1	Category I	R41	Severe Irritant	Guerriero et al. (2004)
Chlorhexidine	55-56-1	100%	Category 1	SCNM	Review Data	Severe Irritant	Balls et al. (1995)
Cyclohexanol	108-93-0	100%	Category 1	Category I	R41	Severe Irritant	Balls et al. (1995)
Dibenzoyl-L-tartaric acid	2743-38-6	100%	Category 1	SCNM	R41	Nonsevere Irritant	Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	100%	Category 2A	Category II	R36	Nonsevere Irritant	Balls et al. (1995)
Dibutyltin chloride	683-18-1	100%	-	-	R41	Severe Irritant	CEC (1991)
3,4-Dichloroaniline hydrochloride (F11)	-	100%	SCNM	SCNM	SCNM	Severe Irritant	Guerriero et al. (2004)
2,6-Dichlorobenzenesulfonyl chloride (F1)	6579-54-0	100%	SCNM	SCNM	SCNM	Severe Irritant	Guerriero et al. (2004)
2,6-Dichlorobenzoyl chloride	4659-45-4	100%	Category 2A	Category II	Review Data	Nonsevere Irritant	Balls et al. (1995)
2,6-Dichloro-5-fluoro-beta-oxo-3-pyridinepropanoate (F16)	96568-04-6	100%	Category 2B	Category III	nonirritant	Nonsevere Irritant	Guerriero et al. (2004)
1-(3,4-Dichlorophenyl)-5-isopropylbiguanide HCl (F6)	537-21-3	100%	Category 1	Category I	R41	Severe Irritant	Guerriero et al. (2004)
3,4-Dimethoxybenzaldehyde (F19)	120-14-9	100%	Nonirritant	Category III	Nonirritant	Nonsevere Irritant	Guerriero et al. (2004)

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2,2-Dimethylbutanoic acid	595-37-9	100%	SCNM	Category I	Review Data	Severe Irritant	Balls et al. (1995)
Dimethyl carbonate (F30)	616-38-6	100%	Nonirritant	Category III	Nonirritant	Severe Irritant	Guerrero et al. (2004)
2,5-Dimethylhexanediol	110-03-2	100%	Category 1	Category I	R41	Nonsevere Irritant	Balls et al. (1995)
Dimethyl sulfoxide	67-68-5	100%	-	-	Nonirritant	Nonsevere Irritant	CEC (1991)
Ethanol	64-17-5	100%	Category 2A	Category III	nonirritant	Severe Irritant	Balls et al. (1995)
Ethyl acetate	141-78-6	100%	Nonirritant	Category III	Nonirritant	Severe Irritant	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	100%	Category 2A	Category II	R36	Nonsevere Irritant	Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	100%	Category 2B	Category III	nonirritant	Severe Irritant	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	100%	Nonirritant	Category III	Nonirritant	Nonsevere Irritant	Balls et al. (1995)
Fluorescein, sodium	518-47-8	100%	-	-	Review Data	Nonsevere irritant	CEC (1991)
p-Fluor-aniline	371-40-4	100%	SCNM	SCNM	Review Data	Severe Irritant	Balls et al. (1995)
Fomesafen, acid form (solid)	72128-02-0	100%	Nonirritant	Category III	Nonirritant	Severe Irritant	Balls et al. (1995)
Glycerol	56-81-5	100%	-	-	Nonirritant	Nonsevere Irritant	CEC (1991)
Glycerol	56-81-5	100%	Nonirritant	Category IV	Nonirritant	Nonsevere Irritant	Balls et al. (1995)
Glycerol (F41)	56-81-5	100%	Nonirritant	Category IV	Nonirritant	Nonsevere Irritant	Guerrero et al. (2004)
n-Hexane	110-54-3	100%	-	-	Nonirritant	Nonsevere Irritant	CEC (1991)
n-Hexanol	111-27-3	100%	Category 2A	Category II	R36	Severe Irritant	Balls et al. (1995)
3-Hydroxy-2-phenyl-4-quinolinecarboxylic acid (F24)	485-89-2	100%	Nonirritant	Category II	Nonirritant	Nonsevere Irritant	Guerrero et al. (2004)
HZA-1	-	Undiluted	Category 1	Category I	R41	Severe irritant	Gettings et al. (1996)
HZB-1	-	25%	Category 1	Category I	R41	Severe irritant	Gettings et al. (1996)
HZC-1	-	25%	Category 1	Category I	R41	Nonsevere irritant	Gettings et al. (1996)
HZD-1	-	25%	Category 2B	Category III	nonirritant	Nonsevere irritant	Gettings et al. (1996)
HZE-1	-	Undiluted	SCNM	Category I	SCNM	Nonsevere irritant	Gettings et al. (1996)
HZF-1	-	Undiluted	Category 1	Category I	R41	Nonsevere irritant	Gettings et al. (1996)
HZG-1	-	25%	Category 1	Category I	R41	Severe irritant	Gettings et al. (1996)
HZH-1	-	Undiluted	Nonirritant	Category IV	Nonirritant	Nonsevere irritant	Gettings et al. (1996)
HZI-1	-	Undiluted	Category 1	Category I	R41	Severe irritant	Gettings et al. (1996)
HZJ-1	-	Undiluted	Nonirritant	Category IV	Nonirritant	Nonsevere irritant	Gettings et al. (1996)
HZK-1	-	Undiluted	Category 1	Category I	R41	Severe irritant	Gettings et al. (1996)
HZL-1	-	Undiluted	Category 1	Category I	R41	Severe irritant	Gettings et al. (1996)
HZM-1	-	25%	Category 1	Category I	R41	Severe irritant	Gettings et al. (1996)
HZN-1	-	25%	Category 1	Category I	R41	Severe irritant	Gettings et al. (1996)

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HZP-1	-	Undiluted	Nonirritant	Category III	Nonirritant	Severe irritant	Gettings et al. (1996)
HZQ-1	-	Undiluted	Nonirritant	Category III	Nonirritant	Nonsevere irritant	Gettings et al. (1996)
HZR-1	-	25%	Category 1	Category I	R41	Nonsevere irritant	Gettings et al. (1996)
HZS-1	-	Undiluted	Category 1	Category I	R41	Severe irritant	Gettings et al. (1996)
HZT-1	-	Undiluted	Nonirritant	Category IV	Nonirritant	Nonsevere irritant	Gettings et al. (1996)
HZU-1	-	25%	Category 2B	Category III	R36	Severe irritant	Gettings et al. (1996)
HZV-1	-	25%	Category 1	Category I	R41	Severe irritant	Gettings et al. (1996)
HZW-1	-	25%	Category 1	Category I	R41	Nonsevere irritant	Gettings et al. (1996)
HZX-1	-	Undiluted	Category 1	Category I	R41	Nonsevere irritant	Gettings et al. (1996)
HZY-1	-	Undiluted	Category 1	Category I	R41	Nonsevere irritant	Gettings et al. (1996)
HZZ-1	-	Undiluted	Nonirritant	Category IV	Nonirritant	Nonsevere irritant	Gettings et al. (1996)
Imidazole	288-32-4	100%	Category 1	Category I	R41	Severe Irritant	Balls et al. (1995)
1H-Indole-2,3-dione (F28)	91-56-5	100%	Nonirritant	Category IV	Nonirritant	Nonsevere Irritant	Guerrero et al. (2004)
Iodine chloride with pyridine (1:1) (F10)	6443-90-9	100%	Category 1	Category I	R41	Severe Irritant	Guerrero et al. (2004)
di-Isopropyl aminoethyl-diphenyl acetamide (F15)	-	100%	Category 2B	Category III	R36	Nonsevere Irritant	Guerrero et al. (2004)
Isopropyl dicyanamide (F9)	35695-36-4	100%	Category 1	Category I	R41	Severe Irritant	Guerrero et al. (2004)
Maneb	12427-38-2	100%	SCNM	Category III	Review Data	Severe Irritant	Balls et al. (1995)
Mebrophen hydramine HCl (F5)	13977-28-1	100%	Category 1	Category I	R41	Severe Irritant	Guerrero et al. (2004)
Mercuric chloride	7546-30-7	100%	-	-	RD	Severe irritant	CEC (1991)
2-Methoxyethanol	109-86-4	100%	-	-	Nonirritant	Severe Irritant	CEC (1991)
1-(2-Methoxyphenyl)piperazine hydrogen sulfate (F2)	-	100%	SCNM	SCNM	SCNM	Severe Irritant	Guerrero et al. (2004)
Methyl acetate	79-20-9	100%	Category 2A	Category II	R36	Severe Irritant	Balls et al. (1995)
6-(Methylamino)-2-pyridine ethanol formate (1:1) (salt) (F17)	-	100%	Nonirritant	Category III	Nonirritant	Severe Irritant	Guerrero et al. (2004)
Methyl cyanoacetate	105-34-0	100%	Category 2A	Category II	R36	Nonsevere Irritant	Balls et al. (1995)
Methylcyclopentane	96-37-7	100%	Nonirritant	Category III	Nonirritant	Nonsevere Irritant	Balls et al. (1995)

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4,4'-Methylenebis-(2,6-di-tert-butylphenol) (F43)	118-82-3	100%	Nonirritant	Category III	Nonirritant	Nonsevere Irritant	Guerrero et al. (2004)
Methyl ethyl ketone	78-93-3	100%	Category 2A	Category III	R36	Severe Irritant	Balls et al. (1995)
Methyl ethyl ketone (F38)	78-93-3	100%	Nonirritant	Category III	Nonirritant	Severe Irritant	Guerrero et al. (2004)
Methyl isobutyl ketone	108-10-1	100%	Nonirritant	Category III	Nonirritant	Severe Irritant	Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	100%	Category 1	Category I	Review Data	Nonsevere Irritant	Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	100%	Category 1	Category I	R41	Severe Irritant	Balls et al. (1995)
2-Nitro-4-propoxyaniline (F23)	-	100%	Nonirritant	Category III	Nonirritant	Nonsevere Irritant	Guerrero et al. (2004)
2-Nitro-4-thiocyananiline (F7)	54029-45-7	100%	Category 1	Category I	R41	Severe Irritant	Guerrero et al. (2004)
2-Nitro-4-thio-N-propylaniline (F21)	54393-89-4	100%	Nonirritant	Category III	Nonirritant	Severe Irritant	Guerrero et al. (2004)
<i>n</i> -Octanol	111-87-5	100%	Category 2A	Category II	R36	Severe Irritant	Balls et al. (1995)
tetra-N-Octylammonium bromide (F8)	14866-33-2	100%	Category 1	Category I	R41	Severe Irritant	Guerrero et al. (2004)
2-(4-Oxopentyl)-1H-isoindole-1,3(2H)-dione (F26)	3197-25-9	100%	Nonirritant	Category III	Nonirritant	Nonsevere Irritant	Guerrero et al. (2004)
(S)-1-Phenyl-N-propylamine (F13)	3789-59-1	100%	SCNM	SCNM	SCNM	Severe Irritant	Guerrero et al. (2004)
Polyethylene glycol 400	25322-68-3	100%	Nonirritant	Category IV	Nonirritant	Severe Irritant	Balls et al. (1995)
Polyethylene glycol 400 (F44)	25322-68-3	100%	Nonirritant	Category IV	Nonirritant	Nonsevere Irritant	Guerrero et al. (2004)
Potassium cyanate	590-28-3	100%	SCNM	SCNM	Review Data	Nonsevere Irritant	Balls et al. (1995)
Promethazine HCl	58-33-3	100%	Category 1	Category I	R41	Severe Irritant	Balls et al. (1995)
iso-Propanol	67-63-0	100%	Category 2A	Category III	Review Data	Severe Irritant	Balls et al. (1995)
Propylene glycol (F42)	57-55-6	100%	Nonirritant	Category IV	Nonirritant	Nonsevere Irritant	Guerrero et al. (2004)
Pyridine	110-86-1	100%	Category 1	Category I	R41	Severe Irritant	Balls et al. (1995)
4,4'-Pyridylpiperidine (F12)	-	100%	SCNM	SCNM	SCNM	Severe Irritant	Guerrero et al. (2004)
Quinacrine	69-05-6	100%	Category 1	Category I	R41	Nonsevere Irritant	Balls et al. (1995)
Silver nitrate	7761-88-8	3% in water	-	-	Review Data	Nonsevere irritant	CEC (1991)

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Sodium dicyanamide (F3)	-	100%	Category 1	Category I	R41	Severe Irritant	Guerrero et al. (2004)
Sodium dodecyl sulfate	151-21-3	100%	-	-	R41	Severe Irritant	CEC (1991)
Sodium hydroxide	1310-73-2	1% in water	-	-	Review Data	Severe irritant	CEC (1991)
Sodium hydroxide (1%)	1310-73-2	1%	Category 2B	Category III	R36	Severe Irritant	Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	10%	Category 1	Category I	R41	Severe Irritant	Balls et al. (1995)
Sodium hydroxide (F31)	1310-73-2	10%	Category 1	Category I	R41	Severe Irritant	Guerrero et al. (2004)
Sodium lauryl sulfate (15 %)	151-21-3	15%	Category 1	Category I	Review Data	Nonsevere Irritant	Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	3%	Nonirritant	Category III	Nonirritant	Nonsevere Irritant	Balls et al. (1995)
Sodium oxalate	62-76-0	100%	Category 1	Category I	R41	Nonsevere Irritant	Balls et al. (1995)
Sodium perborate tetrahydrate	10486-00-7	100%	Category 1	Category I	R41	Nonsevere Irritant	Balls et al. (1995)
4,4'-Sulfonylbisbenzenamine (F25)	80-08-0	100%	Nonirritant	Category IV	Nonirritant	Nonsevere Irritant	Guerrero et al. (2004)
Toluene	108-88-3	100%	-	-	Nonirritant	Nonsevere Irritant	CEC (1991)
Toluene	108-88-3	100%	Nonirritant	Category III	Nonirritant	Severe Irritant	Balls et al. (1995)
Toluene (F40)	108-88-3	100%	Nonirritant	Category III	Nonirritant	Nonsevere Irritant	Guerrero et al. (2004)
Triacetin	102-76-1	100%	-	-	Nonirritant	Nonsevere Irritant	CEC (1991)
Tributyltin chloride	688-73-3	100%	-	-	R41	Severe Irritant	CEC (1991)
Trichloroacetic acid (3%)	76-03-9	3%	Nonirritant	Category III	Nonirritant	Nonsevere Irritant	Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	30%	Category 1	Category I	R41	Severe Irritant	Balls et al. (1995)
Trichloroacetic acid (F32)	76-03-9	30%	Category 1	Category I	R41	Severe Irritant	Guerrero et al. (2004)
Triethanolamine	102-71-6	100%	-	-	Nonirritant	Nonsevere Irritant	CEC (1991)
Triton X-100 (10 %)	9002-93-1	10%	Category 1	Category II	R41	Severe Irritant	Balls et al. (1995)
Triton X-100 (5 %)	9002-93-1	5%	Category 2A	Category III	R36	Severe Irritant	Balls et al. (1995)
Tween 20	9005-64-5	100%	Nonirritant	Category III	Nonirritant	Nonsevere Irritant	Balls et al. (1995)

Abbreviations: SCNM = study criteria not met to allow for a classification

Bolded substances are included in the Expanded Data Set