

SMILES

O=C1N(N(C(=O)C1CCCC)c1ccccc1)c1ccccc1
Clc1ccc(NC(=NC(=NCCCCCN=C(N=C(Nc2ccc(Cl)cc2)N)N)N)N)cc1
OC(CO)CO
[Br-].[N+](CCCCCCCCCCCCCCCC)(C)(C)C
Cl.S1c2c(N(c3c1ccccc3)CC(N(C)C)C)cccc2
[Na+].[Na+].O=C([O-])C(=O)[O-]
OCC
OC(C)C
O=C(C)C
S(=O)(C)C
Cl.Clc1cc2nc3c(cc(OC)cc3)c(NC(CCCN(CC)CC)C)c2cc1
ClC(Cl)(Cl)C(O)=O
OCC(C)C
O=C(CC)C
O(C(=O)C)C
O1C(CO)C(O)C(O)C(O)C1=O
O=C1NN(CC1)c1ccccc1
Oc1ccc(cc1)C(OCCC)=O
Oc1ccccc1N
c1c(C)c(ccc1C)C
ClC(CCl)CCl
C1CCCC1C
O1CCCC1=O
OCCN(CCO)CCO
OCC(CCCC)CC
O(C(=O)CC#N)C
OCC=C
O=[N+](O)CCC
O=C(CC(C)C)C
c1ccccc1C
OC1CCCCC1
O=C1CCCCC1
O(CCO)C
o1cccc1
OC(CCC(O)(C)C)(C)C
C(CCC)CC
O(CCO)CC
n1ccccc1
OCCCCC
O(CCCC)CCO
OCCCCCCCC
c12c(cc3c(c1)cccc3)cccc2
[Cl-].O(CCOCC[N+](Cc1ccccc1)(C)C)c1ccc(cc1)C(CC(C)(C)C)(C)C
O=C(CC(=O)C)C
O(C(=O)C)CCCC
ClC(Cl)(Cl)SN1C(=O)C2C(CC=CC2)C1=O

[Br-].[n+]₁(cccc1)CCCCCCCCCCCCCCC
O(C(=O)C)CC
O(C(=O)CC(=O)C)CC
S(OCCCCCCCCCCC)(=O)(=O)[O-].[Na+]
[nH]₁ccnc1
[Na+].OC1CC2C(C3CCC(C(CCC(=O)[O-])C)C13C)CCC1CC(O)CCC12C
N1c2c(Cc3c1cccc3)cccc2
OC(=O)C[N+](C)(C)C.[OH-]
OC(=O)C(CC)(C)C
O(C(=O)C(C(=O)C)C)CC
OC(=O)c1ccc(cc1)C=O
N(C(N=C(N)N)=N)(C)C
S=C1NC=CC=N1
P(OCc1cccc1)(OCc1cccc1)(O)=O
Clc1cc(Cl)c(S(=O)(=O)N)cc1C(O)=O
O(C(=O)c1cccc1)C(C(OC(=O)c1cccc1)C(O)=O)C(O)=O
O(C(=O)C(C)(C)C)CC
Clc1cccc(Cl)c1C(Cl)=O
S(O)(O)(=O)=O.n1c(N)c(N)c(nc1N)N
[Na+].O=C([O-])CN(CCCCCCCCCC)C
[Cl-].[NH+](Cc1cccc1)(C)C
O(CCCCCCCCCC)CCO
O(CCO)c1ccc(cc1)C(CC(C)(C)C)(C)C
O1CC(OCCO)C(OCCO)C1C(OCCO)COCCOC(=O)CCCCCCCCC
[Mn+2].S=C([S-])NCCNC(=S)[S-]
C12CC(CC1=CC)C=C2
[K+].[K+].O.O.O.C(=O)CN(CCN(CC(=O)[O-])CC(O)=O)CC(=O)[O-]
O(CCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCO)CCOCCOCCOCCOCCOCCOCCOCCO
Clc1cc(ccc1O)c1cc(C(=O)NS(=O)(=O)C([N+](=O)[O-])cc1)C(F)(F)F

Name	CASRN	Composite GHS category
Phenylbutazone	50339	0 Nonirritant
Chlorhexidine	55561	1 Category 1
Glycerol	56815	0 Nonirritant
Hexadecyltrimethylammonium bromide	57090	1 Category 1
Promethazine hydrochloride	58333	1 Category 1
Sodium oxalate	62760	1 Category 1
Ethanol	64175	1 Category 2A
Isopropanol	67630	1 Category 2A
Acetone	67641	1 Category 2A
Dimethyl sulfoxide	67685	0 Nonirritant
Quinacrine	69056	1 Category 1
Trichloroacetic acid (3%)	76039	1 Category 1
Isobutanol	78831	1 Category 2A
Methyl ethyl ketone	78933	1 Category 2A
Methyl acetate	79209	1 Category 2A
Gluconolactone	90802	0 Nonirritant
1-Phenyl-3-pyrazolidone	92433	0 Nonirritant
Propyl-4-hydroxybenzoate	94133	0 Nonirritant
2-Aminophenol	95556	0 Nonirritant
1,2,4-Trimethylbenzene	95636	0 Nonirritant
1,2,3-Trichloropropane	96184	0 Nonirritant
Methylcyclopentane	96377	0 Nonirritant
Butyrolactone	96480	1 Category 2A
Triethanolamine	102716	0 Nonirritant
2-Ethyl-1-hexanol	104767	1 Category 2A
Methyl cyanoacetate	105340	1 Category 2A
Allyl alcohol	107186	1 Category 2A
1-Nitropropane	108032	0 Nonirritant
Methyl isobutyl ketone	108101	0 Nonirritant
Toluene	108883	0 Nonirritant
Cyclohexanol	108930	1 Category 1
Cyclohexanone	108941	0 Nonirritant
2-Methoxyethanol	109864	0 Nonirritant
Furan	110009	0 Nonirritant
2,5-Dimethylhexanediol	110032	1 Category 1
Hexane	110543	0 Nonirritant
2-Ethoxyethanol	110805	0 Nonirritant
Pyridine	110861	1 Category 1
n-Hexanol	111273	1 Category 2A
Butyl cellusolve	111762	1 Category 1
n-Octanol	111875	1 Category 2B
Anthracene	120127	0 Nonirritant
Benzethonium chloride	121540	1 Category 1
2,4-Pentanedione	123546	0 Nonirritant
Butyl acetate	123864	0 Nonirritant
Captan 90 concentrate	133062	1 Category 1

Cetylpyridinium bromide (10%)	140727	1 Category 1
Ethyl acetate	141786	0 Nonirritant
Ethyl acetoacetate	141979	0 Nonirritant
Sodium lauryl sulfate (15 %)	151213	1 Category 1
Imidazole	288324	1 Category 1
Deoxycholic acid, sodium salt	302954	1 Category 2A
Iminodibenzyl	494199	0 Nonirritant
Betaine monohydrate	590476	0 Nonirritant
2,2-Dimethylbutanoic acid	595379	1 SCNM
Ethyl-2-methylacetoacetate	609143	0 Category 2B
4-Carboxybenzaldehyde	619669	1 Category 2A
Dimethylbiguanide	657249	0 Nonirritant
2-Mercaptopyrimidine	1450857	0 Nonirritant
Dibenzyl phosphate	1623081	1 Category 2A
2,4-Dichloro-5-sulfamoylbenzoic acid	2736234	0 Nonirritant
Benzoyl-L-tartaric acid	2743386	1 Category 1
Ethyl trimethyl acetate	3938952	0 Nonirritant
2,6-Dichlorobenzoyl chloride	4659454	1 Category 2A
Tetraaminopyrimidine sulfate	5392289	0 Nonirritant
N-Lauroylsarcosine, sodium salt	7631983	0 Category 2B
Benzalkonium chloride (100 %)	8001545	1 Category 1
BRIJ-35	9002920	0 Nonirritant
Triton X-100 (10%)	9002931	1 Category 2A
Tween 20	9005645	0 Nonirritant
Maneb	12427382	0 SCNM
5-Ethylidene-2-norbornene	16219753	0 Nonirritant
EDTA, di-potassium salt	25102129	0 Nonirritant
Polyethylene glycol 400	25322683	0 Nonirritant
Fomesafen	72128020	0 Nonirritant

US EPA category	EU category
Category IV	Nonirritant
SCNM	SCNM
Category IV	Nonirritant
Category I	R41
Category I	R41
Category I	R41
Category II	Nonirritant
Category III	SCNM
Category II	R36
Category III	Nonirritant
Category I	R41
Category I	R41
Category II	R36
Category III	R36
Category II	R36
Category IV	Nonirritant
Category III	Nonirritant
Category III	Nonirritant
Category IV	Nonirritant
Category III	Nonirritant
Category III	Nonirritant
Category III	Nonirritant
Category II	R36
Category IV	Nonirritant
Category II	R36
Category II	R36
Category III	R36
Category IV	Nonirritant
Category III	Nonirritant
Category III	Nonirritant
Category I	R41
Category III	Nonirritant
Category III	Nonirritant
Category III	Nonirritant
Category I	R41
Category IV	Nonirritant
Category III	Nonirritant
Category I	R41
Category II	R36
Category II	R41
Category III	R36
Category IV	Nonirritant
Category I	R41
Category III	Nonirritant
Category III	Nonirritant
Category I	R41

Category I	R41
Category III	Nonirritant
Category III	Nonirritant
Category I	R36
Category I	R41
Category II	R36
Category III	Nonirritant
Category III	Nonirritant
Category I	SCNM
Category III	Nonirritant
Category II	R36
Category III	Nonirritant
Category IV	Nonirritant
Category II	R36
Category III	Nonirritant
Category I	R41
Category III	Nonirritant
Category II	SCNM
Category III	Nonirritant
Category III	Nonirritant
Category I	R41
Category IV	Nonirritant
Category II	R41
Category III	Nonirritant
Category III	SCNM
Category IV	Nonirritant
Category III	Nonirritant
Category IV	Nonirritant
Category III	Nonirritant