Cyclophosphamide

Other names:

(.+/-.)-Cyclophosphamide
(2S)-N,N-bis(2-chloroethyl)-2-oxo-1-oxa-3-aza-2$l^{5}-phosphacyclohexan-2-amine
(RS)-Cyclophosphamide
2-(Bis(2-chloroethyl)amino)-2H-1,3,2-oxazaphosphorine 2-oxide
2-[Bis(2-chloroethylamino)]-tetrahydro-2H-1,3,2-oxazaphosphorine-2-oxide
2-[bis(2-chloroethyl)amino]tetrahydro-2H-1,3,2-oxazophosphorine-2-oxide
2H-1,3,2-Oxazaphosphorin-2-amine, N,N-bis(2-chloroethyl)tetrahydro-, 2-oxide
2H-1,3,2-Oxazaphosphorine, 2-(bis(2-chloroethyl)amino)tetrahydro-,2-oxide
Asta B 518
B 518
Bis(2-chloroethyl)phosphoramide cyclic propanolamide ester
CB 4564
CP
CPA
CTX
CY
Clafen
Claphene
Cycloblastin
Cyclophosphamid
Cyclophosphamidum
Cyclophosphan
Cyclophosphane
Cyclophosphoramide
Cyclostin
Cyklofosfamid
Cytophosphan
Cytoxan
Endoxan
Endoxan R
Endoxan-Asta
Endoxana
Endoxanal
Endoxane
Enduxan
Genoxal
Hexadrin
Mitoxan
N,N-Bis(2-chloroethyl)-N',O-propylenephosphoric acid ester diamide
N,N-Bis(2-chloroethyl)tetrahydro-2H-1,3,2-oxazaphosphorin-2-amine-2-oxide

N,N-Bis(«beta»-chloroethyl)-N',O-trimethylenephosphoric acid ester diamide
N,N-Bis(Â«betaÂ»-chloroethyl)-N',O-trimethylenephosphoric acid ester diamide
N,N-Bis-(«beta»-chloraethyl)-N',O-propylen-phosphorsaeure-ester-diamid
N,N-Bis-(Â«betaÂ»-chloraethyl)-N',O-propylen-phosphorsaeure-ester-diamid
N,N-Di(2-chloroethyl)-N,O-propylene-phosphoric acid ester diamide
NCI-C04900
NSC 26271
Neosar
Phosphorodiamidic acid, N,N-bis(2-chloroethyl)-N'-(3-hydroxypropyl)-, intramol. ester
Procytox
RCRA Waste number U058
SK 20501
Semdoxan
Sendoxan
Senduxan
Zyklophosphamid

Inchi: InChI=1S/C7H15Cl2N2O2P/c8-2-5-11(6-3-9)14(12)10-4-1-7-13-14/h1-7H2,(H,10,12)
InchiKey: CMSMOCZEIVJLDB-UHFFFAOYSA-N
Formula: C7H15Cl2N2O2P
SMILES: O=P1(N(CCCl)CCCl)NCCCO1
Mol. weight [g/mol]: 261.09
CAS: 50-18-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.81		Aqueous Solubility Prediction Method
logp	1.884		Crippen Method
mcvol	175.270	ml/mol	McGowan Method
tf	318.98	K	Aqueous Solubility Prediction Method
tf	323.52 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	33.13	kJ/mol	322.60	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50180&Units=SI

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point