Uracil Mustard

Other names:	2,4(1H,3H)-Pyrimidinedione, 5-[bis(2-chloroethyl)amino]-
	Uracil, 5-[bis(2-chloroethyl)amino]-
	Aminouracil mustard
	Chlorethaminacil
	Demethyldopan
	Desmethyldopan
	ENT 50439
	Nordopan
	NSC-34462
	U-8344
	Uracillost
	Uracilmostaza
	Uramustin
	Uramustine
	2,6-Dihydroxy-5-[bis(2-chloroethyl)amino]pyrimidine
	5-[Bis(2-chloroethyl)amino]uracil
	5-[Di(«beta»-chloroethyl)amino]uracil
	CB-4835
	NCI-C04820
	SK-19849
	Uracil nitrogen mustard
	5-(Bis(2-chlorethyl)amino)-2,4(1H,3H)pyrimidinedione
	5-(Di(2-chloroethyl)amino)uracil
	5-(Bis(2-chloroethyl)amino)-2,4(1H,3H)pyrimidinedione
	5-N,N-Bis(2-chloroethyl)aminouracil
	Rcra waste number U237
Inchi:	InChI=1S/C8H11Cl2N3O2/c9-1-3-13(4-2-10)6-5-11-8(15)12-7(6)14/h5H,1-4H2,(H2,11,12
InchiKey:	IDPUKCWIGUEADI-UHFFFAOYSA-N
Formula:	C8H11Cl2N3O2
SMILES:	O=c1[nH]cc(N(CCCl)CCCl)c(=O)[nH]1
Mol. weight [g/mol]:	252.10
CAS:	66-75-1

Physical Properties

Property code	Value	Unit	Source
log10ws	0.19		Crippen Method

logp	-0.617		Crippen Method
mcvol	165.980	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66751&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume