Altretamine

Other names:	1,3,5-Triazine-2,4,6-triamine, N,N,N',N',N'',N''-hexamethyl-
	1,3,5-tris(dimethylamino)-s-triazine
	2,4,6-Tris(Dimethylamino)-s-triazine
	2,4,6-Tris(dimethylamino)-1,3,5-triazine
	ENT 50852
	HMM
	HTM
	HXM
	Hemel
	Hexalen
	Hexamethylmelamine
	Hexastat
	Melamine, hexamethyl-
	N,N,N',N',N'',N''-Hexamethyl-1,3,5-triazine-2,4,6-triamine
	NC 195
	NCI-C50259
	NSC 13875
	s-Triazine, 2,4,6-tris(dimethylamino)-
Inchi:	InChI=1S/C9H18N6/c1-13(2)7-10-8(14(3)4)12-9(11-7)15(5)6/h1-6H3
InchiKey:	UUVWYPNAQBNQJQ-UHFFFAOYSA-N
Formula:	C9H18N6
SMILES:	CN(C)c1nc(N(C)C)nc(N(C)C)n1
Mol. weight [g/mol]:	210.28
CAS:	645-05-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.36		Aqueous Solubility Prediction Method
log10ws	-3.36		Estimated Solubility Method
logp	0.070		Crippen Method
mcvol	173.790	ml/mol	McGowan Method
tf	444.35 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	23.01	kJ/mol	444.40	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
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C645056&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