Propazine

Other names:	1,3,5-Triazine-2,4-diamine, 6-chloro-N,N'-bis(1-methylethyl)-
	1,3,5-Triazine-2,4-diamine, 6-chloro-N2,N4-bis(1-methylethyl)-
	2,4-Bis(isopropylamino)-6-chloro-s-triazine
	2,4-Bis(propylamino)-6-chlor-1,3,5-triazine
	2,4-bis(1-methylethyl-amino)-6-chloro-s-triazine
	2-Chlor-4,6-bis(isopropylamino)-s-triazine
	2-Chloro-4,6-bis(isopropylamino)-1,3,5-triazine
	2-Chloro-4,6-bis(isopropylamino)-s-triazine
	6-Chloro-N,N'-(1-methylethyl)-[1,3,5]triazine-2,4-diamine
	6-Chloro-N,N'-bis(1-methylethyl)-1,3,5-triazine-2,4-diamine
	6-Chloro-N,N'-di(1-methylethyl)-[1,3,5]triazine-2,4-diamine
	6-Chloro-N,N'-diisopropyl-1,3,5-triazine-2,4-diyldiamine
	6-chloro-N,N'-di(propan-2-yl)-1,3,5-triazine-2,4-diamine
	G 30028
	Geigy 30,028
	Gesamil
	Milo-pro
	Milogard
	NSC 26002
	Plantulin
	Primatol P
	Propasin
	Propazin
	Propazine (Herbicide)
	Prozinex
	s-Triazine, 2-chloro-4,6-bis(isopropylamino)-
Inchi:	InChI=1S/C9H16ClN5/c1-5(2)11-8-13-7(10)14-9(15-8)12-6(3)4/h5-6H,1-4H3,(H2,11,12,1
InchiKey:	WJNRPILHGGKWCK-UHFFFAOYSA-N
Formula:	C9H16ClN5
SMILES:	CC(C)Nc1nc(Cl)nc(NC(C)C)n1
Mol. weight [g/mol]:	229.71
CAS:	139-40-2

Physical Properties

Property code	Value	Unit	Source
chs	-5688.30 ± 8.90	kJ/mol	NIST Webbook

hfs	-163.60 ± 9.70	kJ/mol	NIST Webbook
log10ws	-4.43		Estimated Solubility Method
log10ws	-4.43		Aqueous Solubility Prediction Method
logp	2.166		Crippen Method
mcvol	176.050	ml/mol	McGowan Method
rinpol	1735.00		NIST Webbook
rinpol	1756.00		NIST Webbook
rinpol	1761.00		NIST Webbook
rinpol	1759.00		NIST Webbook
rinpol	1706.00		NIST Webbook
rinpol	1756.00		NIST Webbook
rinpol	1753.88		NIST Webbook
rinpol	1763.13		NIST Webbook
rinpol	1735.00		NIST Webbook
rinpol	1767.32		NIST Webbook
rinpol	1777.68		NIST Webbook
rinpol	1763.13		NIST Webbook
rinpol	1776.59		NIST Webbook
rinpol	1733.00		NIST Webbook
rinpol	1733.00		NIST Webbook
rinpol	1753.88		NIST Webbook
rinpol	1770.00		NIST Webbook
ripol	2633.00		NIST Webbook
ripol	2633.00		NIST Webbook
ripol	2659.00		NIST Webbook
ripol	2633.00		NIST Webbook
tf	489.60 ± 0.20	K	NIST Webbook
tf	490.52 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	41.87	kJ/mol	490.30	NIST Webbook
hsubt	125.10	kJ/mol	363.00	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=C139402&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
hfs:	Solid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tf:	Normal melting (fusion) point

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