Simetryn

Other names:	1,3,5-Triazine-2,4-diamine, N,N'-diethyl-6-(methylthio)-
	2,4-Bis(ethylamino)-6-(methylmercapto)-s-triazine
	2,4-Bis(ethylamino)-6-(methylthio)-s-triazine
	2,4-Bis(ethylamino)-6-methylthio-1,3,5-triazine
	2-(Methylmercapto)-4,6-bis(ethylamino)-s-triazine
	2-(Methylthio)-4,6-bis(ethylamino)-s-triazine
	2-Methylthio-4,6-bis(ethylamino)-1,3,5-triazine
	2-Methylthio-4,6-bis(ethylamino)-1,3,5-triazine (simetryn)
	2-Methylthio-4,6-bis(monoethylamino)-2-triazine
	4,6-Bis(ethylamino)-2-(methylthio)-1,3,5-triazine
	Cymetrin
	G 32911
	Gy-Bon
	N,N'-Diethyl-6-(methylthio)-1,3,5-triazine-2,4-diamine
	N,N'-diethyl-6-methylsulfanyl-1,3,5-triazine-2,4-diamine
	NSC 163051
	Simetryne
	Symetryne
	s-Triazine, 2,4-bis(ethylamino)-6-(methylthio)-
Inchi:	InChI=1S/C8H15N5S/c1-4-9-6-11-7(10-5-2)13-8(12-6)14-3/h4-5H2,1-3H3,(H2,9,10,11,12
InchiKey:	MGLWZSOBALDPEK-UHFFFAOYSA-N
Formula:	C8H15N5S
SMILES:	CCNc1nc(NCC)nc(SC)n1
Mol. weight [g/mol]:	213.30
CAS:	1014-70-6

Physical Properties

Property code	Value	Unit	Source
hfus	24.00	kJ/mol	Vapor Pressures and Standard Molar Sublimation Enthalpies of Three 6-Methylthio-2,4-di(alkylamino)-1,3,5-triazi Derivatives: Simetryn, Ametryn, and Terbutryn
hvap	115.00 ± 4.00	kJ/mol	NIST Webbook
hvap	120.00 ± 6.00	kJ/mol	NIST Webbook
log10ws	-2.68		Aqueous Solubility Prediction Method

logp	1.457		Crippen Method
mcvol	166.070	ml/mol	McGowan Method
rinpol	1902.00		NIST Webbook
rinpol	1910.00		NIST Webbook
rinpol	1899.00		NIST Webbook
rinpol	1906.00		NIST Webbook
rinpol	1878.00		NIST Webbook
rinpol	1844.00		NIST Webbook
rinpol	1843.00		NIST Webbook
rinpol	1843.00		NIST Webbook
rinpol	1878.00		NIST Webbook
rinpol	1902.00		NIST Webbook
ripol	2915.00		NIST Webbook
ripol	2915.00		NIST Webbook
ripol	2937.00		NIST Webbook
ripol	2915.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	24.00	kJ/mol	353.20	NIST Webbook
hsubt	101.30	kJ/mol	339.00	NIST Webbook
hvapt	88.00 ± 4.00	kJ/mol	461.00	NIST Webbook
hvapt	83.70 ± 1.30	kJ/mol	453.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.54180e+01
Coeff. B	-1.21876e+04
Temperature range (K), min.	484.97
Temperature range (K), max.	606.15

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Vapor Pressures and Standard Molar Sublimation Enthalpies of Three 6-Methylthio-2,4-di(alkylamino)-1,3,5-triazine Derivatives: Simetryn, Ametryn, and Terbutryn:	https://www.doi.org/10.1021/je600580r
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=C1014706&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices