Ametryn

Other names:	1,3,5-Triazine-2,4-diamine, N-ethyl-N'-(1-methylethyl)-6-(methylthio)-
	2-(Ethylamino)-4-(isopropylamino)-6-(methylmercapto)-s-triazine
	2-(Ethylamino)-4-(isopropylamino)-6-(methylthio)-s-triazine
	2-(Methylmercapto)-4-(ethylamino)-6-(isopropylamino)-s-triazine
	2-(Methylmercapto)-4-(isopropylamino)-6-(ethylamino)-s-triazine
	2-(Methylthio)-4-(ethylamino)-6-(isopropylamino)-s-triazine
	2-Ethylamino-4-isopropylamino-6-methylthio-1,3,5-triazine
	2-ethylamino-4-isopropylamino-6-methylthio-s-triazine
	2-methylthio-4-ethylamino-6-isopropylamino-1,3,5-triazine
	A 1093
	Amephyt
	Ametrex
	Ametrine
	Ametryne
	Cemerin
	Crisatrine
	Doruplant
	Evik
	G 34162
	Gesapax
	Mebatryne
	N-Ethyl-N'-(1-methylethyl)-6-(methylthio)-1,3,5-triazine-2,4-diamine
	N-Ethyl-N'-isopropyl-6-methylthio-1,3,5-triazine-2,4-diamine
	N-ethyl-N'-(1-methylethyl)-6-methylthio-1,3,5-triazine-2,4-diamine
	NSC 163044
	Primatol Z 80
	Trinatox D
	s-Triazine, 2-(ethylamino)-4-(isopropylamino)-6-(methylthio)-
Inchi:	InChI=1S/C9H17N5S/c1-5-10-7-12-8(11-6(2)3)14-9(13-7)15-4/h6H,5H2,1-4H3,(H2,10,11
InchiKey:	RQVYBGPQFYCBGX-UHFFFAOYSA-N
Formula:	C9H17N5S
SMILES:	CCNc1nc(NC(C)C)nc(SC)n1
Mol. weight [g/mol]:	227.33
CAS:	834-12-8

Physical Properties

Property code	Value	Unit	Source

chs	-6510.80 ± 4.20	kJ/mol	NIST Webbook
hf	38.50 ± 6.30	kJ/mol	NIST Webbook
hfs	-63.10 ± 5.00	kJ/mol	NIST Webbook
hfus	26.00	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	118.00 ± 4.00	kJ/mol	NIST Webbook
hvap	125.00 ± 6.00	kJ/mol	NIST Webbook
log10ws	-3.04		Estimated Solubility Method
log10ws	-3.04		Aqueous Solubility Prediction Method
logp	1.846		Crippen Method
mcvol	180.160	ml/mol	McGowan Method
rinpol	1911.00		NIST Webbook
rinpol	1869.00		NIST Webbook
rinpol	1911.00		NIST Webbook
rinpol	1882.00		NIST Webbook
rinpol	1882.00		NIST Webbook
rinpol	1911.00		NIST Webbook
rinpol	1907.00		NIST Webbook
rinpol	1912.00		NIST Webbook
rinpol	1916.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1872.00		NIST Webbook
ripol	2837.00		NIST Webbook
ripol	2837.00		NIST Webbook
ripol	2859.00		NIST Webbook
ripol	2837.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	26.00	kJ/mol	359.10	NIST Webbook
hsubt	100.90	kJ/mol	363.00	NIST Webbook
hvapt	91.00 ± 4.00	kJ/mol	466.00	NIST Webbook
hvapt	84.90 ± 1.30	kJ/mol	453.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.54113e+01
Coeff. B	-1.21346e+04
Temperature range (K), min.	482.99
Temperature range (K), max.	603.72

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C834128&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
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

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
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