Terbutryn

Other names:	1,3,5-Triazine-2,4-diamine, N-(1,1-dimethylethyl)-N'-ethyl-6-(methylthio)-
	2-Methylmercapto-4-ethylamino-6-tert-butylamino-1,3,5-triazine (terbutryn)
	2-Methylthio-4-ethylamino-6-tert-butylamino-s-triazine
	2-Tert.-butylamino-4-ethylamino-6-methylthio-[1,3,5]triazin
	2-Tert.-butylamino-4-ethylamino-6-methylthio-[1,3,5]triazine
	2-tert-Butylamino-4-ethylamino-6-methylmercapto-s-triazine
	2-tert-Butylamino-4-ethylamino-6-methylthio-1,3,5-triazine
	2-tert-Butylamino-4-ethylamino-6-methylthio-s-triazine
	2-tert.Butylamino-4-aethylamino-6-methylthio-1,3,5-triazin
	4-Aethylamino-2-tert-butylamino-6-methylthio-s-triazin
	A 1866
	Athado
	Clarosan
	GS 14260
	HS-14260
	Igran
	Igran 50
	Igran 500
	N-(1,1-Dimethylethyl)-N'-ethyl-6-(methylthio)-1,3,5-triazine-2,4-diamine
	Plantonit
	Prebane
	Saterb
	Short-stop E
	Shortstop
	Terbutrex
	Terbutrin
	Terbutryne
	s-Triazine, 2-(tert-butylamino)-4-(ethylamino)-6-(methylthio)-
Inchi:	InChI=1S/C10H19N5S/c1-6-11-7-12-8(15-10(2,3)4)14-9(13-7)16-5/h6H2,1-5H3,(H2,11,1
InchiKey:	IROINLKCQGIITA-UHFFFAOYSA-N
Formula:	C10H19N5S
SMILES:	CCNc1nc(NC(C)(C)C)nc(SC)n1
Mol. weight [g/mol]:	241.36
CAS:	886-50-0

Physical Properties

Property code	Value	Unit	Source

hfus	21.00	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	111.00 ± 4.00	kJ/mol	NIST Webbook
hvap	115.00 ± 7.00	kJ/mol	NIST Webbook
log10ws	-4.00		Aqueous Solubility Prediction Method
log10ws	-4.00		Estimated Solubility Method
logp	2.236		Crippen Method
mcvol	194.250	ml/mol	McGowan Method
rinpol	1906.00		NIST Webbook
rinpol	1940.00		NIST Webbook
rinpol	1912.00		NIST Webbook
rinpol	1902.00		NIST Webbook
rinpol	1945.00		NIST Webbook
rinpol	1939.00		NIST Webbook
rinpol	1944.00		NIST Webbook
rinpol	1945.00		NIST Webbook
rinpol	1944.00		NIST Webbook
rinpol	1939.00		NIST Webbook
rinpol	1910.00		NIST Webbook
rinpol	1940.00		NIST Webbook
rinpol	1906.00		NIST Webbook
rinpol	1902.00		NIST Webbook
ripol	2793.00		NIST Webbook
ripol	2812.00		NIST Webbook
ripol	2793.00		NIST Webbook
tf	376.98 ± 0.20	K	NIST Webbook
tf	377.53	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	21.00	kJ/mol	376.10	NIST Webbook
hfust	21.42	kJ/mol	375.90	NIST Webbook
hvapt	87.00 ± 5.00	kJ/mol	467.00	NIST Webbook
hvapt	83.20 ± 1.00	kJ/mol	452.00	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C886500&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion 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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tf:	Normal melting (fusion) point