Metribuzin

Other names:	1,2,4-Triazin-5(4H)-one, 4-amino-6-(1,1-dimethylethyl)-3-(methylthio)-
	1,2,4-Triazin-5-one, 4-amino-6-tert-butyl-3-(methylthio)-
	3-Methylthio-4-amino-6-tert-butyl-1,2,4-triazin-5-one
	4-Amino-6-(1,1-dimethylethyl)-3-(methylthio)-1,2,4-triazin-5(4H)-one
	4-Amino-6-tert-butyl-3-(methylthio)-1,2,4-triazin-5-one
	4-Amino-6-tert-butyl-3-(methylthio)-as-triazin-5(4H)-one
	4-Amino-6-tert-butyl-3-methylthio-as-triazin-5-one
	As-Triazin-5(4H)-one, 4-amino-6-tert-butyl-3-(methylthio)-
	BAY 6159
	BAY 6159 H
	BAY 61597
	BAY 94337
	BAY DIC 1468
	BAYER 94337
	Bayer 6159
	Bayer 6159H
	Bayer 6443H
	DIC 1468
	Lexone
	Lexone 4L
	Lexone 75DF
	Lexone DF
	Metoribuzine
	Metribuzine
	Sencor
	Sencor 4F
	Sencor 4L
	Sencor 75DF
	Sencor DF
	Sencoral
	Sencorer
	Sencorex
	Sencorex L.F.
	Senkor
	Triazin-5(4H)-one, 4-amino-6-tert-butyl-3-(methylthio)-
	Zenkor
Inchi:	InChI=1S/C8H14N4OS/c1-8(2,3)5-6(13)12(9)7(14-4)11-10-5/h9H2,1-4H3
InchiKey:	FOXFZRUHNHCZPX-UHFFFAOYSA-N
Formula:	C8H14N4OS
SMILES:	CSc1nnc(C(C)(C)C)c(=O)n1N

Mol. weight [g/mol]: 214.29
CAS: 21087-64-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.25		Aqueous Solubility Prediction Method
log10ws	-2.25		Estimated Solubility Method
logp	0.372		Crippen Method
mcvol	161.960	ml/mol	McGowan Method
rinpol	1873.00		NIST Webbook
rinpol	1835.00		NIST Webbook
rinpol	1849.00		NIST Webbook
rinpol	1819.00		NIST Webbook
rinpol	1882.00		NIST Webbook
rinpol	1888.00		NIST Webbook
rinpol	1813.00		NIST Webbook
rinpol	1819.00		NIST Webbook
rinpol	1873.00		NIST Webbook
tf	399.94 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	18.00	kJ/mol	399.40	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21087649&Units=SI
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

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
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point