Terbumeton

Other names:	1,3,5-Triazine-2,4-diamine, N-(1,1-dimethylethyl)-N'-ethyl-6-methoxy-
	1,3,5-Triazine-2,4-diamine, N2-(1,1-dimethylethyl)-N4-ethyl-6-methoxy-
	2-Methoxy-4-tert-butylamino-6-aethylamino-s-triazin
	2-tert-Butylamino-4-ethylamino-6-methoxy-1,3,5-triazine
	2-tert-Butylamino-4-ethylamino-6-methoxy-s-triazine
	A 2591
	Caragard
	GS 14259
	Karagard
	N-tert-Butyl-N'-ethyl-6-methoxy-[1,3,5]triazin-2,4-diamin
	N-tert-Butyl-N'-ethyl-6-methoxy-[1,3,5]triazin-2,4-diamine
	Terbuthylon
	Terbutone
	Tribunil G 14259
	s-Triazine, 2-(tert-butylamino)-4-(ethylamino)-6-methoxy-
	s-Triazine, 2-ethylamino-4-tert-butylamino-6-methoxy
	s-Triazine, 2-ethylamino-4-tert.-butylamino-6-methoxy
Inchi:	InChI=1S/C10H19N5O/c1-6-11-7-12-8(15-10(2,3)4)14-9(13-7)16-5/h6H2,1-5H3,(H2,11,1
InchiKey:	BCQMBFHBDZVHKU-UHFFFAOYSA-N
Formula:	C10H19N5O
SMILES:	CCN=c1nc(NC(C)(C)C)[nH]c(OC)n1
Mol. weight [g/mol]:	225.29
CAS:	33693-04-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.24		Aqueous Solubility Prediction Method
log10ws	-3.24		Estimated Solubility Method
logp	0.462		Crippen Method
mcvol	183.770	ml/mol	McGowan Method
ripol	2598.00		NIST Webbook
ripol	2570.00		NIST Webbook
ripol	2570.00		NIST Webbook
ripol	2570.00		NIST Webbook
tf	396.65	K	Aqueous Solubility Prediction Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33693048&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

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices
tf:	Normal melting (fusion) point

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