Tricyclazole

Other names:	1,2,4-Triazolo[3,4-b]benzothiazole, 5-methyl-
	5-Methyl-1,2,4-triazole(3,4-b)benzothiazole
	5-Methyl-1,2,4-triazolo[3,4-b]benzothiazole
	5-methyl-1,2,4-triazolo[3,4-b]benzo-1,3-thiazole
	BIM
	Beam
	Blascide
	EL 291
	Elanco 291
	MTB
	Sivic
	Tricyclazone
	Tricyclozole
	s-Triazolo(3,4-b)benzothiazole, 5-methyl-
Inchi:	InChI=1S/C9H7N3S/c1-6-3-2-4-7-8(6)12-5-10-11-9(12)13-7/h2-5H,1H3
InchiKey:	DQJCHOQLCLEDLL-UHFFFAOYSA-N
Formula:	C9H7N3S
SMILES:	Cc1cccc2sc3nncn3c12
Mol. weight [g/mol]:	189.24
CAS:	41814-78-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.07		Aqueous Solubility Prediction Method
log10ws	-2.07		Estimated Solubility Method
logp	2.252		Crippen Method
mcvol	129.880	ml/mol	McGowan Method
rinpol	2185.00		NIST Webbook
tf	460.49 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

hfust	24.07	kJ/mol	460.20	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41814782&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

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

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