

Tebuthiuron

Other names:	Urea, N-[5-(1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl]-N,N'-dimethyl- Urea, 1-(5-tert-butyl-1,3,4-thiadiazol-2-yl)-1,3-dimethyl- EL 103 Spike Urea, 1-(5-(t-butyl)-1,3,4-thiadiazol-2-yl)-1,3-dimethyl- Brulan 1-(5-tert-Butyl-1,3,4-thiadiazol-2-yl)-3-dimethylharnstoff 1-(5-tert-Butyl-1,3,4-thiadiazol-2-yl)-1,3-dimethylurea N-(5-(1,1-Dimethylaethyl)-1,3,4-thiadiazol-2-yl)-N,N'-dimethylharnstoff Graslan Perflan Perfmid Preflan Prefmid Tebulan Tiurolole Bushwacker N-(5-tert-Butyl-1,3,4-thiadiazol-2-yl)-N,N'-dimethylurea N-[5-(1,1-Dimethylethyl)-1,3,4-thiadiazol-2-yl]-NN'-dimethylurea Graslan 250 brush bullets Spike 80W
Inchi:	InChI=1S/C9H16N4OS/c1-9(2,3)6-11-12-8(15-6)13(5)7(14)10-4/h1-5H3,(H,10,14)
InchiKey:	HBPKDSDFLXWQAE-UHFFFAOYSA-N
Formula:	C9H16N4OS
SMILES:	CNC(=O)N(C)c1nnc(C(C)(C)C)s1
Mol. weight [g/mol]:	228.31
CAS:	34014-18-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.34		Crippen Method
logp	1.611		Crippen Method
mccvol	176.050	ml/mol	McGowan Method
tf	436.61 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	29.48	kJ/mol	435.30	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34014181&Units=SI

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
tf:	Normal melting (fusion) point

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