Thiazole, 4,5-dimethyl-2-(2-methylpropyl)-

Other names:	4,5-Dimethyl-2-isobutylthiazole
	2-iso-Butyl-4,5-dimethylthiazole
	2-(2-methylpropyl)-4,5-dimethylthiazole
	Thiazole, 2-isobutyl-4,5-dimethyl
Inchi:	InChI=1S/C9H15NS/c1-6(2)5-9-10-7(3)8(4)11-9/h6H,5H2,1-4H3
InchiKey:	NSVPHVLZAKJSGV-UHFFFAOYSA-N
Formula:	C9H15NS
SMILES:	Cc1nc(CC(C)C)sc1C
Mol. weight [g/mol]:	169.29
CAS:	53498-32-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.34		Crippen Method
logp	2.958		Crippen Method
mcvol	144.540	ml/mol	McGowan Method
rinpol	1207.00		NIST Webbook
rinpol	1224.00		NIST Webbook
rinpol	1186.00		NIST Webbook
rinpol	1183.00		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1193.00		NIST Webbook
rinpol	1225.00		NIST Webbook
rinpol	1207.00		NIST Webbook
rinpol	1186.00		NIST Webbook
rinpol	1215.00		NIST Webbook
rinpol	1193.00		NIST Webbook
ripol	1514.00		NIST Webbook
ripol	1517.00		NIST Webbook
ripol	1514.00		NIST Webbook
ripol	1514.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C53498321&Units=SI

Legend

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