Thiazole, 2-butyl-4,5-dimethyl-

Other names:	2-n-Butyl-4,5-dimethylthiazole
	2-Butyl-4,5-dimethyl-thiazole
Inchi:	InChI=1S/C9H15NS/c1-4-5-6-9-10-7(2)8(3)11-9/h4-6H2,1-3H3
InchiKey:	OHJFDYDPHXVQBC-UHFFFAOYSA-N
Formula:	C9H15NS
SMILES:	CCCCc1nc(C)c(C)s1
Mol. weight [g/mol]:	169.29
CAS:	76572-48-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	3.103		Crippen Method
mcvol	144.540	ml/mol	McGowan Method
rinpol	1287.00		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1287.00		NIST Webbook
ripol	1658.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1658.00		NIST Webbook
ripol	1600.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C76572480&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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