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

Physical Properties

Property code	Value	Unit	Source
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
tf	241.85	K	Cheméo Relay (1.0)

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C76572480&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tf:	Normal melting (fusion) point