Thiazole, 2,4-dimethyl-5-propyl-

Other names: 2,4-Dimethyl-5-propylthiazole
Inchi: InChI=1S/C8H13NS/c1-4-5-8-6(2)9-7(3)10-8/h4-5H2,1-3H3
InchiKey: BNONKJGVAXAEFW-UHFFFAOYSA-N
Formula: C8H13NS
SMILES: CCCc1sc(C)nc1C
Mol. weight [g/mol]: 155.26
CAS: 41981-70-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.17		Crippen Method
logp	2.712		Crippen Method
mcvol	130.450	ml/mol	McGowan Method
rinpol	1157.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1153.00		NIST Webbook
ripol	1515.00		NIST Webbook
ripol	1515.00		NIST Webbook
ripol	1515.00		NIST Webbook

Sources

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=C41981708&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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