

Thiazole, 2,5-dimethyl-4-propyl

Inchi: InChI=1S/C8H13NS/c1-4-5-8-6(2)10-7(3)9-8/h4-5H2,1-3H3
InchiKey: VIWROTZGLFXXMS-UHFFFAOYSA-N
Formula: C8H13NS
SMILES: CCCc1nc(C)sc1C
Mol. weight [g/mol]: 155.26

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
ripol	1515.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R317656&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

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<https://www.chemeo.com/cid/64-160-3/Thiazole-2-5-dimethyl-4-propyl.pdf>

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