2-Heptyl-4,5-dimethylthiazole

Inchi: InChI=1S/C12H21NS/c1-4-5-6-7-8-9-12-13-10(2)11(3)14-12/h4-9H2,1-3H3
InchiKey: PSZGSWWQPRJONL-UHFFFAOYSA-N
Formula: C12H21NS
SMILES: CCCCCCCc1nc(C)c(C)s1
Mol. weight [g/mol]: 211.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.84		Crippen Method
logp	4.273		Crippen Method
mcvol	186.810	ml/mol	McGowan Method
rinpol	1588.00		NIST Webbook
rinpol	1575.00		NIST Webbook
rinpol	1588.00		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=R329996&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