2-Octyl-4,5-dimethylthiazole

Inchi: InChI=1S/C13H23NS/c1-4-5-6-7-8-9-10-13-14-11(2)12(3)15-13/h4-10H2,1-3H3
InchiKey: HGRFDZGIRVFJRV-UHFFFAOYSA-N
Formula: C13H23NS
SMILES: CCCCCCCCc1nc(C)c(C)s1
Mol. weight [g/mol]: 225.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.26		Crippen Method
logp	4.663		Crippen Method
mcvol	200.900	ml/mol	McGowan Method
rinpol	1691.00		NIST Webbook
rinpol	1678.00		NIST Webbook
rinpol	1692.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R330015&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