2-Hexyl-4,5-dimethylthiazole

Inchi: InChI=1S/C11H19NS/c1-4-5-6-7-8-11-12-9(2)10(3)13-11/h4-8H2,1-3H3
InchiKey: KVNSTYMROSOFEA-UHFFFAOYSA-N
Formula: C11H19NS
SMILES: CCCCCCc1nc(C)c(C)s1
Mol. weight [g/mol]: 197.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.42		Crippen Method
logp	3.883		Crippen Method
mcvol	172.720	ml/mol	McGowan Method
rinpol	1485.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1473.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R330000&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

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