2-heptyl-4-methyl-thiazole

Inchi: InChI=1S/C11H19NS/c1-3-4-5-6-7-8-11-12-10(2)9-13-11/h9H,3-8H2,1-2H3
InchiKey: WMGXEJPIBZDULA-UHFFFAOYSA-N
Formula: C11H19NS
SMILES: CCCCCCCc1nc(C)cs1
Mol. weight [g/mol]: 197.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.37		Crippen Method
logp	3.964		Crippen Method
mcvol	172.720	ml/mol	McGowan Method
rinpol	1532.00		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=R497584&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