4-ethyl-2-heptyl-5-methyl-thiazole

Inchi: InChI=1S/C13H23NS/c1-4-6-7-8-9-10-13-14-12(5-2)11(3)15-13/h4-10H2,1-3H3
InchiKey: SSLICXPSYONSAZ-UHFFFAOYSA-N
Formula: C13H23NS
SMILES: CCCCCCCc1nc(CC)c(C)s1
Mol. weight [g/mol]: 225.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.17		Crippen Method
logp	4.527		Crippen Method
mcvol	200.900	ml/mol	McGowan Method
rinpol	1634.00		NIST Webbook
rinpol	1635.00		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=R497871&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.