2-hexyl-4-ethyl-5-methyl-thiazole

Inchi: InChI=1S/C12H21NS/c1-4-6-7-8-9-12-13-11(5-2)10(3)14-12/h4-9H2,1-3H3
InchiKey: HUPMTZMZEGOTOW-UHFFFAOYSA-N
Formula: C12H21NS
SMILES: CCCCCCc1nc(CC)c(C)s1
Mol. weight [g/mol]: 211.37

Physical Properties

Property code	Value	Unit	Source
logp	4.137		Crippen Method
mcvol	186.810	ml/mol	McGowan Method
rinpol	1533.00		NIST Webbook
rinpol	1534.00		NIST Webbook
rinpol	1534.00		NIST Webbook
rinpol	1533.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R497920&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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