5-ethyl-4-methyl-2-octyl-thiazole

Inchi:	InChI=1S/C14H25NS/c1-4-6-7-8-9-10-11-14-15-12(3)13(5-2)16-14/h4-11H2,1-3H3
InchiKey:	KABDBXXFTIHONZ-UHFFFAOYSA-N
Formula:	C14H25NS
SMILES:	CCCCCCCCc1nc(C)c(CC)s1
Mol. weight [g/mol]:	239.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.59		Crippen Method
logp	4.917		Crippen Method
mcvol	214.990	ml/mol	McGowan Method
rinpol	1760.00		NIST Webbook
rinpol	1762.00		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=R498334&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

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