4,5-dimethyl-2-nonyl-thiazole

Inchi:	InChI=1S/C14H25NS/c1-4-5-6-7-8-9-10-11-14-15-12(2)13(3)16-14/h4-11H2,1-3H3
InchiKey:	TUBGURMWJWGLPY-UHFFFAOYSA-N
Formula:	C14H25NS
SMILES:	CCCCCCCCCc1nc(C)c(C)s1
Mol. weight [g/mol]:	239.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.68		Crippen Method
logp	5.053		Crippen Method
mcvol	214.990	ml/mol	McGowan Method
rinpol	1795.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R497777&Units=SI

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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