

4-ethyl-5-methyl-2-nonyl-thiazole

Inchi:	InChI=1S/C15H27NS/c1-4-6-7-8-9-10-11-12-15-16-14(5-2)13(3)17-15/h4-12H2,1-3H3
InchiKey:	VFCKTBMFRTVJPG-UHFFFAOYSA-N
Formula:	C15H27NS
SMILES:	CCCCCCCCc1nc(CC)c(C)s1
Mol. weight [g/mol]:	253.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.01		Crippen Method
logp	5.307		Crippen Method
mcvol	229.080	ml/mol	McGowan Method
rinsol	1839.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R498032&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinsol:	Non-polar retention indices

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