

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

Inchi: InChI=1S/C15H27NS/c1-4-6-7-8-9-10-11-12-15-16-13(3)14(5-2)17-15/h4-12H2,1-3H3
InchiKey: YPKROAYRSLYFEP-UHFFFAOYSA-N
Formula: C15H27NS
SMILES: CCCCCCCCCc1nc(C)c(CC)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
rinpol	1864.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R498309&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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<https://www.chemeo.com/cid/31-056-5/5-ethyl-4-methyl-2-nonyl-thiazole.pdf>

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