4-ethyl-2-hexyl-thiazole

Inchi:	InChI=1S/C11H19NS/c1-3-5-6-7-8-11-12-10(4-2)9-13-11/h9H,3-8H2,1-2H3
InchiKey:	GEAVQUKRDITJTP-UHFFFAOYSA-N
Formula:	C11H19NS
SMILES:	CCCCCCc1nc(CC)cs1
Mol. weight [g/mol]:	197.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.27		Crippen Method
logp	3.828		Crippen Method
mcvol	172.720	ml/mol	McGowan Method
rinpol	1516.00		NIST Webbook
rinpol	1516.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R497935&Units=SI
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

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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