

2-hexyl-4-methyl-thiazole

Inchi:	InChI=1S/C10H17NS/c1-3-4-5-6-7-10-11-9(2)8-12-10/h8H,3-7H2,1-2H3
InchiKey:	JAKJZOOTXAIFDV-UHFFFAOYSA-N
Formula:	C10H17NS
SMILES:	CCCCCCc1nc(C)cs1
Mol. weight [g/mol]:	183.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.95		Crippen Method
logp	3.574		Crippen Method
mcvol	158.630	ml/mol	McGowan Method
rinsol	1426.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R497608&Units=SI

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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<https://www.chemeo.com/cid/39-494-1/2-hexyl-4-methyl-thiazole.pdf>

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