

4-methyl-2-pentyl-thiazole

Inchi:	InChI=1S/C10H17NS/c1-3-5-6-7-10-11-9(4-2)8-12-10/h8H,3-7H2,1-2H3
InchiKey:	ZHOPDZKIOONDFH-UHFFFAOYSA-N
Formula:	C10H17NS
SMILES:	CCCCC1nc(CC)cs1
Mol. weight [g/mol]:	183.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.86		Crippen Method
logp	3.438		Crippen Method
mcvol	158.630	ml/mol	McGowan Method
rinpol	1322.00		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=R498136&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

Latest version available from:

<https://www.chemeo.com/cid/58-793-8/4-methyl-2-pentyl-thiazole.pdf>

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