

2-Butyl-5-methylthiazole

Other names: Thiazole, 2-butyl-5-methyl-
Inchi: InChI=1S/C8H13NS/c1-3-4-5-8-9-6-7(2)10-8/h6H,3-5H2,1-2H3
InchiKey: FCMSADORJFIRBT-UHFFFAOYSA-N
Formula: C8H13NS
SMILES: CCCCC1ncc(C)s1
Mol. weight [g/mol]: 155.26
CAS: 52414-85-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.11		Crippen Method
logp	2.794		Crippen Method
mcvol	130.450	ml/mol	McGowan Method
ripol	1738.00		NIST Webbook
ripol	1738.00		NIST Webbook
ripol	1738.00		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=C52414854&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
ripol: Polar retention indices

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