

Thiazole-5-ethanol, 4-methyl, acetate

Other names: 2-(4-methylthiazol-5-yl)ethyl acetate
Inchi: InChI=1S/C8H11NO2S/c1-6-8(12-5-9-6)3-4-11-7(2)10/h5H,3-4H2,1-2H3
InchiKey: CRTWCWNPLKVVXIX-UHFFFAOYSA-N
Formula: C8H11NO2S
SMILES: CC(=O)OCCc1scnc1C
Mol. weight [g/mol]: 185.24
CAS: 656-53-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.97		Crippen Method
logp	1.557		Crippen Method
mcvol	137.890	ml/mol	McGowan Method
rinpol	1368.00		NIST Webbook
ripol	2077.00		NIST Webbook
ripol	2077.00		NIST Webbook

Sources

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=C656531&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

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

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