

5-Acetyl-4-methylthiazole

Other names:	Thiazole, 5-acetyl-4-methyl
Inchi:	InChI=1S/C6H7NOS/c1-4-6(5(2)8)9-3-7-4/h3H,1-2H3
InchiKey:	MBLHLRLBSIWLMG-UHFFFAOYSA-N
Formula:	C6H7NOS
SMILES:	CC(=O)c1scnc1C
Mol. weight [g/mol]:	141.19
CAS:	38205-55-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.13		Crippen Method
logp	1.654		Crippen Method
mcvol	103.840	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38205559&Units=SI
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

Legend

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

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