2-Acetyl-5-methylthiazole

Inchi: InChI=1S/C6H7NOS/c1-4-3-7-6(9-4)5(2)8/h3H,1-2H3
InchiKey: ZGOBPVBSAXXNES-UHFFFAOYSA-N
Formula: C6H7NOS
SMILES: CC(=O)c1ncc(C)s1
Mol. weight [g/mol]: 141.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.13		Crippen Method
logp	1.654		Crippen Method
mcvol	103.840	ml/mol	McGowan Method
rinpol	1076.00		NIST Webbook
ripol	1685.00		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=R331578&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