

5-Acetyl-2,4-dimethylthiazole

Other names:	2,4-Dimethyl-5-acetylthiazole Ethanone, 1-(2,4-dimethyl-5-thiazolyl)- 5-Acetyl-2,4-dimethylthiazole Thiazole, 5-acetyl-2,4-dimethyl 1-(2,4-dimethylthiazol-5-yl)ethan-1-one
Inchi:	InChI=1S/C7H9NOS/c1-4-7(5(2)9)10-6(3)8-4/h1-3H3
InchiKey:	BLQOKWQUTLNKON-UHFFFAOYSA-N
Formula:	C7H9NOS
SMILES:	CC(=O)c1sc(C)nc1C
Mol. weight [g/mol]:	155.22
CAS:	38205-60-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.61		Crippen Method
logp	1.963		Crippen Method
mcvol	117.930	ml/mol	McGowan Method
ripol	1217.00		NIST Webbook
ripol	1835.00		NIST Webbook
ripol	1835.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C38205606&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
ripol: Polar retention indices

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<https://www.chemeo.com/cid/27-737-4/5-Acetyl-2-4-dimethylthiazole.pdf>

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