

2-Acetyl-4-methylthiazole

Other names:	Thiazole, 2-acetyl-4-methyl 4-methyl-2-acetylthiazole Ethanone, 1-(4-methyl-2-thiazolyl)- 1-(5-methyl-1,3-thiazol-2-yl)ethanone
Inchi:	InChI=1S/C6H7NOS/c1-4-3-9-6(7-4)5(2)8/h3H,1-2H3
InchiKey:	QPUIPSFYQGKAFL-UHFFFAOYSA-N
Formula:	C6H7NOS
SMILES:	CC(=O)c1nc(C)cs1
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	1094.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1118.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1136.00		NIST Webbook
ripol	1668.00		NIST Webbook
ripol	1668.00		NIST Webbook
ripol	1685.00		NIST Webbook
ripol	1665.00		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=C7533075&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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