

5-Acetylpyrimidine

Inchi:	InChI=1S/C6H6N2O/c1-5(9)6-2-7-4-8-3-6/h2-4H,1H3
InchiKey:	COTYNDRSENVEFI-UHFFFAOYSA-N
Formula:	C6H6N2O
SMILES:	CC(=O)c1cncnc1
Mol. weight [g/mol]:	122.12
CAS:	10325-70-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.66		Crippen Method
logp	0.679		Crippen Method
mcvol	93.170	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10325709&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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<https://www.chemeo.com/cid/98-611-5/5-Acetylpyrimidine.pdf>

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