

1-Acetyl-4,5-dihydro-1H-pyrazole

Inchi:	InChI=1S/C5H8N2O/c1-5(8)7-4-2-3-6-7/h3H,2,4H2,1H3
InchiKey:	OWQPLIVCAIEJFS-UHFFFAOYSA-N
Formula:	C5H8N2O
SMILES:	CC(=O)N1CCC=N1
Mol. weight [g/mol]:	112.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.31		Crippen Method
logp	0.224		Crippen Method
mcvol	87.680	ml/mol	McGowan Method
rinpola	1159.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373426&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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