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
rinpol	1159.00		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=U373426&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