3-Acetyl-1-methylpyrrole

Inchi: InChI=1S/C7H9NO/c1-6(9)7-3-4-8(2)5-7/h3-5H,1-2H3
InchiKey: SZYIVZGXCXFXDN-UHFFFAOYSA-N
Formula: C7H9NO
SMILES: CC(=O)c1ccn(C)c1
Mol. weight [g/mol]: 123.15
CAS: 932-62-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.42		Crippen Method
logp	1.228		Crippen Method
mcvol	101.580	ml/mol	McGowan Method
rinpol	1195.00		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=C932627&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

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