N-Acetylpyrrole

Other names: Pyrrole, 1-acetyl
Inchi: InChI=1S/C6H7NO/c1-6(8)7-4-2-3-5-7/h2-5H,1H3
InchiKey: OMYOJDLCFAUIHN-UHFFFAOYSA-N
Formula: C6H7NO
SMILES: CC(=O)n1cccc1
Mol. weight [g/mol]: 109.13
CAS: 609-41-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.59		Crippen Method
logp	1.148		Crippen Method
mcvol	87.490	ml/mol	McGowan Method
rinpol	957.00		NIST Webbook
rinpol	957.00		NIST Webbook
rinpol	948.00		NIST Webbook
ripol	1554.00		NIST Webbook
ripol	1576.00		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=C609416&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