

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/ci990307I

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

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