

N-Acetylpyrrolidone

Other names:	N-Acetyl-2-pyrrolidone N-Acetyl-2-pyrrolidinone 2-Pyrrolidinone, 1-acetyl- 1-acetylpyrrolidin-2-one
Inchi:	InChI=1S/C6H9NO2/c1-5(8)7-4-2-3-6(7)9/h2-4H2,1H3
InchiKey:	YLHUPYSUKYAIBW-UHFFFAOYSA-N
Formula:	C6H9NO2
SMILES:	CC(=O)N1CCCC1=O
Mol. weight [g/mol]:	127.14
CAS:	932-17-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.35		Crippen Method
logp	0.155		Crippen Method
mcvol	97.660	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	392.00 ± 1.00	K	2.70	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C932172&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure

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