Pyrrolidine, 1-acetyl-

Other names:	N-Acetylpyrrolidine
	1-Acetylpyrrolidine
	N-Acetypyrrolidine
	Pyrrolidine, N-acetyl
	Acetylpyrrolidine
Inchi:	InChI=1S/C6H11NO/c1-6(8)7-4-2-3-5-7/h2-5H2,1H3
InchiKey:	LNWWQYYLZVZXKS-UHFFFAOYSA-N
Formula:	C6H11NO
SMILES:	CC(=O)N1CCCC1
Mol. weight [g/mol]:	113.16
CAS:	4030-18-6

Physical Properties

Property code	Value	Unit	Source
affp	925.40	kJ/mol	NIST Webbook
basg	894.40	kJ/mol	NIST Webbook
log10ws	-0.57		Crippen Method
logp	0.629		Crippen Method
mcvol	96.090	ml/mol	McGowan Method
rinpol	1128.00		NIST Webbook
rinpol	1128.00		NIST Webbook
ripol	1766.00		NIST Webbook
ripol	1766.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	379.00 ± 1.00	K	2.00	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=C4030186&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
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
tbrp:	Boiling point at reduced pressure

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