

Pyrrolidine, 1-(cyanoacetyl)-

Other names:	1-Cyanoacetylpyrrolidine N-Cyanoacetylpyrrolidine
Inchi:	InChI=1S/C7H10N2O/c8-4-3-7(10)9-5-1-2-6-9/h1-3,5-6H2
InchiKey:	VEUDVNNBYRZBV-UHFFFAOYSA-N
Formula:	C7H10N2O
SMILES:	N#CCC(=O)N1CCCC1
Mol. weight [g/mol]:	138.17
CAS:	14227-95-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.86		Crippen Method
logp	0.522		Crippen Method
mcvol	111.560	ml/mol	McGowan Method

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=C14227953&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/49-625-4/Pyrrolidine-1-cyanoacetyl.pdf>

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