1-Pyrrolidinylacetonitrile

Other names:	1-Pyrrolidineacetonitrile
	Pyrrolidinoacetonitrile
	Pyrroldinoacetonitrile
	1-Cyanomethylpyrrolidine
	N-Pyrrolidinoacetonitrile
	pyrrolidine-1-acetonitrile
Inchi:	InChI=1S/C6H10N2/c7-3-6-8-4-1-2-5-8/h1-2,4-6H2
InchiKey:	NPRYXVXVLCYBNS-UHFFFAOYSA-N
Formula:	C6H10N2
SMILES:	N#CCN1CCCC1
Mol. weight [g/mol]:	110.16
CAS:	29134-29-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.67		Crippen Method
logp	0.606		Crippen Method
mcvol	95.900	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29134290&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