

Pyrrolidinoacetonitrile

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

Physical Properties

Property code	Value	Unit	Source
hf	126.28	kJ/mol	Cheméo Relay (1.0)
hvap	53.32	kJ/mol	Cheméo Relay (1.0)
logp	0.606		Crippen Method
mcvol	95.900	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29134290&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

hf:	Enthalpy of formation at standard conditions
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h_{vap}:	Enthalpy of vaporization at standard conditions
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume

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