

1-PIPERIDINECARBONITRILE

Other names:	Piperidine, 1-carbonitrile- piperidinocarbonitrile
Inchi:	InChI=1S/C6H10N2/c7-6-8-4-2-1-3-5-8/h1-5H2
InchiKey:	NVPICXQHSYQKGM-UHFFFAOYSA-N
Formula:	C6H10N2
SMILES:	N#CN1CCCCC1
Mol. weight [g/mol]:	110.16

Physical Properties

Property code	Value	Unit	Source
affp	876.70	kJ/mol	NIST Webbook
basg	846.10	kJ/mol	NIST Webbook
hf	95.50	kJ/mol	Cheméo Relay (1.0)
logp	0.953		Crippen Method
mcvol	95.900	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1530876&Units=SI>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
hf:	Enthalpy of formation at standard conditions
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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