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