

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

CAS: 1530-87-6

Physical Properties

Property code	Value	Unit	Source
affp	876.70	kJ/mol	NIST Webbook
basg	846.10	kJ/mol	NIST Webbook
log10ws	-1.16		Crippen Method
logp	0.953		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=C1530876&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

Legend

affp: Proton affinity

basg: Gas basicity

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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