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/ci990307l
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