

2-Piperidinobenzonitrile

Inchi:	InChI=1S/C12H14N2/c13-10-11-6-2-3-7-12(11)14-8-4-1-5-9-14/h2-3,6-7H,1,4-5,8-9H2
InchiKey:	MEBVSLKZSAIGK-UHFFFAOYSA-N
Formula:	C12H14N2
SMILES:	N#Cc1ccccc1N1CCCCC1
Mol. weight [g/mol]:	186.25
CAS:	72752-52-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.88		Crippen Method
logp	2.549		Crippen Method
mcvol	156.680	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72752524&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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