

Piperidine, 1,2,6-trimethyl-, cis-

Inchi:	InChI=1S/C8H17N/c1-7-5-4-6-8(2)9(7)3/h7-8H,4-6H2,1-3H3/t7-,8+
InchiKey:	COSHJOZVKGAYBP-OCAPTIKFSA-N
Formula:	C8H17N
SMILES:	CC1CCCC(C)N1C
Mol. weight [g/mol]:	127.23
CAS:	2439-13-6

Physical Properties

Property code	Value	Unit	Source
ie	7.77 ± 0.05	eV	NIST Webbook
log10ws	-1.86		Crippen Method
logp	1.879		Crippen Method
mcvol	122.700	ml/mol	McGowan Method

Sources

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=C2439136&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

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

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<https://www.chemeo.com/cid/13-159-1/Piperidine-1-2-6-trimethyl-cis.pdf>

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