

Piperidine, 1-hexyl

Other names:	N-n-hexylpiperidine 1-Hexyl piperidine
Inchi:	InChI=1S/C11H23N/c1-2-3-4-6-9-12-10-7-5-8-11-12/h2-11H2,1H3
InchiKey:	BBYSGWAYRRMWOW-UHFFFAOYSA-N
Formula:	C11H23N
SMILES:	CCCCCN1CCCCC1
Mol. weight [g/mol]:	169.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.89		Crippen Method
logp	3.053		Crippen Method
mcvol	164.970	ml/mol	McGowan Method
rinpol	1220.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1220.00		NIST Webbook
ripol	1342.00		NIST Webbook
ripol	1342.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R222063&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices

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