

Piperidine, 1-hexyl-3-methyl

Inchi: InChI=1S/C12H25N/c1-3-4-5-6-9-13-10-7-8-12(2)11-13/h12H,3-11H2,1-2H3
InchiKey: VVZBHHVBQAFFQP-UHFFFAOYSA-N
Formula: C12H25N
SMILES: CCCCCCN1CCCC(C)C1
Mol. weight [g/mol]: 183.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.07		Crippen Method
logp	3.299		Crippen Method
mcvol	179.060	ml/mol	McGowan Method
rinpol	1274.00		NIST Webbook
rinpol	1274.00		NIST Webbook
ripol	1375.00		NIST Webbook
ripol	1375.00		NIST Webbook

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=R222098&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

Latest version available from:

<https://www.chemeo.com/cid/26-896-9/Piperidine-1-hexyl-3-methyl.pdf>

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