

Piperidine, 1,2,6-trimethyl-

Other names: 1,2,6-Trimethylpiperidine
Inchi: InChI=1S/C8H17N/c1-7-5-4-6-8(2)9(7)3/h7-8H,4-6H2,1-3H3
InchiKey: COSHJOZVKGAYBP-UHFFFAOYSA-N
Formula: C8H17N
SMILES: CC1CCCC(C)N1C
Mol. weight [g/mol]: 127.23
CAS: 669-81-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.86		Crippen Method
logp	1.879		Crippen Method
mcvol	122.700	ml/mol	McGowan Method
rinpol	909.00		NIST Webbook
rinpol	909.00		NIST Webbook
ripol	1050.00		NIST Webbook
ripol	1050.00		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=C669818&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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<https://www.chemeo.com/cid/59-542-5/Piperidine-1-2-6-trimethyl.pdf>

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