

1,3-Dimethyl-pyrrolidine

Other names: Pyrrolidine, 1,3-dimethyl
Inchi: InChI=1S/C6H13N/c1-6-3-4-7(2)5-6/h6H,3-5H2,1-2H3
InchiKey: IGNFGXAWDQJGP-UHFFFAOYSA-N
Formula: C6H13N
SMILES: CC1CCN(C)C1
Mol. weight [g/mol]: 99.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.56		Crippen Method
logp	0.958		Crippen Method
mcvol	94.520	ml/mol	McGowan Method
rinpol	716.00		NIST Webbook
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rinpol	716.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=R405580&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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