

1,3,4-Trimethyl-pyrrolidine

Inchi: InChI=1S/C7H15N/c1-6-4-8(3)5-7(6)2/h6-7H,4-5H2,1-3H3
InchiKey: SIBLCLDNTGUERI-UHFFFAOYSA-N
Formula: C7H15N
SMILES: CC1CN(C)CC1C
Mol. weight [g/mol]: 113.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.73		Crippen Method
logp	1.204		Crippen Method
mcvol	108.610	ml/mol	McGowan Method
rinpol	799.00		NIST Webbook
rinpol	799.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R405575&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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

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