

1-Isopropyl-azetidine

Inchi: InChI=1S/C6H13N/c1-6(2)7-4-3-5-7/h6H,3-5H2,1-2H3
InchiKey: UMPRRBSYZVDQTH-UHFFFAOYSA-N
Formula: C6H13N
SMILES: CC(C)N1CCC1
Mol. weight [g/mol]: 99.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.91		Crippen Method
logp	1.101		Crippen Method
mcvol	94.520	ml/mol	McGowan Method
rinpol	615.00		NIST Webbook
rinpol	615.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R405644&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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<https://www.chemeo.com/cid/77-799-1/1-Isopropyl-azetidine.pdf>

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