

1-Azabicyclo[3.1.0]hexane

Inchi: InChI=1S/C5H9N/c1-2-5-4-6(5)3-1/h5H,1-4H2
InchiKey: QRDSKDAGXMWBID-UHFFFAOYSA-N
Formula: C5H9N
SMILES: C1CC2CN2C1
Mol. weight [g/mol]: 83.13
CAS: 285-76-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.39		Crippen Method
logp	0.464		Crippen Method
mcvol	69.570	ml/mol	McGowan Method
tb	381.50 ± 1.50	K	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=C285767&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature

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<https://www.chemeo.com/cid/77-707-2/1-Azabicyclo-3-1-0-hexane.pdf>

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