

1-tert-Butyl-pyrrolidine

Inchi: InChI=1S/C8H17N/c1-8(2,3)9-6-4-5-7-9/h4-7H2,1-3H3
InchiKey: WNMQSIGDRWCJMO-UHFFFAOYSA-N
Formula: C8H17N
SMILES: CC(C)(C)N1CCCC1
Mol. weight [g/mol]: 127.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.75		Crippen Method
logp	1.881		Crippen Method
mcvol	122.700	ml/mol	McGowan Method
rinpol	905.00		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=R405679&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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<https://www.chemeo.com/cid/34-493-7/1-tert-Butyl-pyrrolidine.pdf>

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