

1-tert-Butyl azetidine

Inchi: InChI=1S/C7H15N/c1-7(2,3)8-5-4-6-8/h4-6H2,1-3H3
InchiKey: XUIKGNBNCYLDNK-UHFFFAOYSA-N
Formula: C7H15N
SMILES: CC(C)(C)N1CCC1
Mol. weight [g/mol]: 113.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.33		Crippen Method
logp	1.491		Crippen Method
mcvol	108.610	ml/mol	McGowan Method
rinpol	794.00		NIST Webbook
rinpol	794.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R405664&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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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