

1-tert-Butyl-aziridine

Inchi: InChI=1S/C6H13N/c1-6(2,3)7-4-5-7/h4-5H2,1-3H3
InchiKey: BBFCEQFUUOTJPD-UHFFFAOYSA-N
Formula: C6H13N
SMILES: CC(C)(C)N1CC1
Mol. weight [g/mol]: 99.17
CAS: 4017-38-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.91		Crippen Method
logp	1.101		Crippen Method
mcvol	94.520	ml/mol	McGowan Method
rinpola	699.00		NIST Webbook
rinpola	699.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C4017383&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpola: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/73-030-7/1-tert-Butyl-aziridine.pdf>

Generated by Cheméo on 2024-04-27 21:34:16.875559505 +0000 UTC m=+16542905.796136836.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.