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
rinpol	699.00		NIST Webbook
rinpol	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
rinpol: Non-polar retention indices