1-Butyl-aziridine

Other names: Aziridine, 1-butyl-
Inchi: InChI=1S/C6H13N/c1-2-3-4-7-5-6-7/h2-6H2,1H3
InchiKey: XIEJPTDTTYFCJM-UHFFFAOYSA-N
Formula: C6H13N
SMILES: CCCCN1CC1
Mol. weight [g/mol]: 99.17
CAS: 1120-85-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.80		Crippen Method
logp	1.102		Crippen Method
mcvol	94.520	ml/mol	McGowan Method
rinpol	754.00		NIST Webbook
rinpol	754.00		NIST Webbook
rinpol	754.00		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=C1120850&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