

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
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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

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