Aziridine, 1-(1-butenyl)-, (E)-

Other names: (E)-1-(1-Butenyl)aziridine
(E)-1-Aziridino-1-butene
1-[(1E)-1-Butenyl]aziridine
Inchi: InChI=1S/C6H11N/c1-2-3-4-7-5-6-7/h3-4H,2,5-6H2,1H3/b4-3+
InchiKey: ZOJXHLVIYWZLQK-ONEGZZNKSA-N
Formula: C6H11N
SMILES: CCC=CN1CC1
Mol. weight [g/mol]: 97.16
CAS: 80839-92-5

Physical Properties

Property code	Value	Unit	Source
ie	7.70	eV	NIST Webbook
ie	7.70	eV	NIST Webbook
ie	8.26	eV	NIST Webbook
ie	8.26	eV	NIST Webbook
log10ws	-1.15		Crippen Method
logp	1.226		Crippen Method
mcvol	90.220	ml/mol	McGowan Method

Sources

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=C80839925&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume