

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

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