

Aziridine, 1,-(1-butenyl)-, (Z)-

Other names:	(Z)-1-(1-Butenyl)aziridine (Z)-1-Aziridino-1-butene
Inchi:	InChI=1S/C6H11N/c1-2-3-4-7-5-6-7/h3-4H,2,5-6H2,1H3/b4-3-
InchiKey:	ZOJXHLYIYWZLQK-ARJAWSKDSA-N
Formula:	C6H11N
SMILES:	CCC=CN1CC1
Mol. weight [g/mol]:	97.16
CAS:	80839-94-7

Physical Properties

Property code	Value	Unit	Source
ie	7.90	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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80839947&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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