Aziridine, 1-(2-methyl-1-propenyl)-

Other names:	1-(2-Methylpropenyl)aziridine
	1-Aziridinoisobutene
Inchi:	InChI=1S/C6H11N/c1-6(2)5-7-3-4-7/h5H,3-4H2,1-2H3
InchiKey:	SUPYAXZORIMKIB-UHFFFAOYSA-N
Formula:	C6H11N
SMILES:	CC(C)=CN1CC1
Mol. weight [g/mol]:	97.16
CAS:	80839-93-6

Physical Properties

Property code	Value	Unit	Source
ie	7.60	eV	NIST Webbook
ie	7.60	eV	NIST Webbook
ie	8.20	eV	NIST Webbook
ie	8.20	eV	NIST Webbook
log10ws	-1.15		Crippen Method
logp	1.226		Crippen Method
mcvol	90.220	ml/mol	McGowan Method

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=C80839936&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

Latest version available from:

https://www.chemeo.com/cid/11-947-8/Aziridine-1-2-methyl-1-propenyl.pdf

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