

1-(2-METHYL-PROPENYL)-AZIRIDINE

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

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
logp	1.226		Crippen Method
mcvol	90.220	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80839936&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/11-947-8/1-2-METHYL-PROPENYL-AZIRIDINE.pdf>

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