

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

Other names:	Pyrrolidine, 1-(2-methylpropenyl)- Isobutyraldehyde pyrrolidine enamine N-(2-Methyl-1-propenyl)pyrrolidine N-Isobutenylpyrrolidine 1-(2-Methyl-1-propenyl)pyrrolidine 1-(2-Methylpropenyl)pyrrolidine 1-Pyrrolidino-2-methylpropene 1-Pyrrolidinoisobutene 2-Methyl-1-pyrrolidinopropene
Inchi:	InChI=1S/C8H15N/c1-8(2)7-9-5-3-4-6-9/h7H,3-6H2,1-2H3
InchiKey:	PAXNHQZTZQFBPC-UHFFFAOYSA-N
Formula:	C8H15N
SMILES:	CC(C)=CN1CCCC1
Mol. weight [g/mol]:	125.21
CAS:	2403-57-8

Physical Properties

Property code	Value	Unit	Source
ie	6.80	eV	NIST Webbook
ie	7.75	eV	NIST Webbook
ie	7.66 ± 0.03	eV	NIST Webbook
log10ws	-1.98		Crippen Method
logp	2.006		Crippen Method
mvol	118.400	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C2403578&Units=SI

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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