Aziridine, 1-(1-propenyl)-, (E)-

Other names:	(E)-1-Propenylaziridine
	(E)-1-Aziridino-1-propene
Inchi:	InChI=1S/C5H9N/c1-2-3-6-4-5-6/h2-3H,4-5H2,1H3/b3-2+
InchiKey:	BEUWPRGCKSXXRV-NSCUHMNNSA-N
Formula:	C5H9N
SMILES:	CC=CN1CC1
Mol. weight [g/mol]:	83.13
CAS:	80839-91-4

Physical Properties

Property code	Value	Unit	Source
ie	7.90	eV	NIST Webbook
ie	8.34	eV	NIST Webbook
log10ws	-0.73		Crippen Method
logp	0.836		Crippen Method
mcvol	76.130	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=C80839914&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume