

Aziridine, 1-methyl-

Other names:	N-Methylaziridine N-Methylethylenimine 1-Methylaziridine 1-Methylethylenimine
Inchi:	InChI=1S/C3H7N/c1-4-2-3-4/h2-3H2,1H3
InchiKey:	XLJQPXVBQNJNLW-UHFFFAOYSA-N
Formula:	C3H7N
SMILES:	CN1CC1
Mol. weight [g/mol]:	57.09
CAS:	1072-44-2

Physical Properties

Property code	Value	Unit	Source
affp	934.80	kJ/mol	NIST Webbook
basg	904.10	kJ/mol	NIST Webbook
ie	8.70	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	9.26	eV	NIST Webbook
log10ws	0.46		Crippen Method
logp	-0.068		Crippen Method
mcvol	52.250	ml/mol	McGowan Method
rinpola	519.00		NIST Webbook
tb	300.70	K	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1072442&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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