

AZIRIDINE, 1-(1-BUTENYL)-, (E)-

Other names:	(E)-1-(1-Butenyl)aziridine (E)-1-Aziridino-1-butene 1-[(1E)-1-Butenyl]aziridine
Inchi:	InChI=1S/C6H11N/c1-2-3-4-7-5-6-7/h3-4H,2,5-6H2,1H3/b4-3+
InchiKey:	ZOJXHLVIYWZLQK-ONEGZZNKSA-N
Formula:	C6H11N
SMILES:	CC/C=C/N1CC1
Mol. weight [g/mol]:	97.16

Physical Properties

Property code	Value	Unit	Source
af	0.3136		Cheméo Relay (1.0)
gf	180.84	kJ/mol	Cheméo Relay (1.0, beta)
hf	90.65	kJ/mol	Cheméo Relay (1.0)
hvap	43.16	kJ/mol	Cheméo Relay (1.0)
ie	7.70	eV	NIST Webbook
ie	8.26	eV	NIST Webbook
ie	8.26	eV	NIST Webbook
ie	7.70	eV	NIST Webbook
logp	1.226		Crippen Method
mcvol	90.220	ml/mol	McGowan Method
pc	3838.59	kPa	Cheméo Relay (1.0, beta)
tb	417.58	K	Cheméo Relay (1.0)
tc	593.82	K	Cheméo Relay (1.0)
tf	203.81	K	Cheméo Relay (1.0)
vc	0.341	m3/kmol	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C80839925&Units=SI>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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