(CH3)2N-CH=N-CH2CN

Inchi: InChI=1S/C5H9N3/c1-8(2)5-7-4-3-6/h5H,4H2,1-2H3
InchiKey: NWYJIMZYZKAACO-UHFFFAOYSA-N
Formula: C5H9N3
SMILES: CN(C)C=NCC#N
Mol. weight [g/mol]: 111.15
CAS: 134166-58-8

Physical Properties

Property code	Value	Unit	Source
affp	948.00	kJ/mol	NIST Webbook
basg	915.50	kJ/mol	NIST Webbook
hf	168.10	kJ/mol	Joback Method
hvap	42.56	kJ/mol	Joback Method
log10ws	-0.01		Crippen Method
logp	0.100		Crippen Method
mcvol	98.350	ml/mol	McGowan Method
pc	2986.06	kPa	Joback Method
tb	505.00	K	Joback Method
tc	713.70	K	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C134166588&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp: Proton affinity

basg:	Gas basicity
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature