

(CH₃)₂N-CH=N-CH₂CH₂CN

Inchi: InChI=1S/C6H11N3/c1-9(2)6-8-5-3-4-7/h6H,3,5H2,1-2H3
InchiKey: HHIMRLAMENYLGA-UHFFFAOYSA-N
Formula: C6H11N3
SMILES: CN(C)C=NCCC#N
Mol. weight [g/mol]: 125.17
CAS: 134166-60-2

Physical Properties

Property code	Value	Unit	Source
affp	980.80	kJ/mol	NIST Webbook
basg	948.30	kJ/mol	NIST Webbook
hf	147.46	kJ/mol	Joback Method
hvap	44.78	kJ/mol	Joback Method
log10ws	-0.43		Crippen Method
logp	0.490		Crippen Method
mcvol	112.440	ml/mol	McGowan Method
pc	2695.80	kPa	Joback Method
tb	527.88	K	Joback Method
tc	733.46	K	Joback Method

Sources

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=C134166602&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp: Proton affinity

basg:	Gas basicity
hf:	Enthalpy of formation at standard conditions
h vap:	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

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