

3,4-Diazanona-3,5-diene

Inchi: InChI=1S/C7H14N2/c1-3-5-6-7-9-8-4-2/h6-7H,3-5H2,1-2H3/b7-6+,9-8+
InchiKey: QXUWPEMSORWKIV-BLHCBFLLSA-N
Formula: C7H14N2
SMILES: CCCC=CN=NCC
Mol. weight [g/mol]: 126.20
CAS: 82946-55-2

Physical Properties

Property code	Value	Unit	Source
hf	-23.37	kJ/mol	Joback Method
hvap	37.80	kJ/mol	Joback Method
ie	8.10	eV	NIST Webbook
log10ws	-2.36		Crippen Method
logp	2.772		Crippen Method
mvol	120.850	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
tb	512.92	K	Joback Method
tc	718.48	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=C82946552&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions

ie:	Ionization energy
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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