2-Methyl-octahydroazocine

Inchi: InChI=1S/C8H17N/c1-8-6-4-2-3-5-7-9-8/h8-9H,2-7H2,1H3
InchiKey: MHEHELVTSIPICT-UHFFFAOYSA-N
Formula: C8H17N
SMILES: CC1CCCCCCN1
Mol. weight [g/mol]: 127.23

Physical Properties

Property code	Value	Unit	Source
gf	104.44	kJ/mol	Joback Method
hf	-128.64	kJ/mol	Joback Method
hfus	13.70	kJ/mol	Joback Method
hvap	40.93	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	1.929		Crippen Method
mcvol	122.700	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
rinpol	916.00		NIST Webbook
tb	459.08	K	Joback Method
tc	685.23	K	Joback Method
tf	285.29	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.07	J/mol×K	459.08	Joback Method
cpg	277.05	J/mol×K	496.77	Joback Method
cpg	296.06	J/mol×K	534.46	Joback Method
cpg	314.11	J/mol×K	572.16	Joback Method
cpg	331.21	J/mol×K	609.85	Joback Method
cpg	347.35	J/mol×K	647.54	Joback Method
cpg	362.53	J/mol×K	685.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R405793&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume