2-Methyl-hexahydroazepine

Inchi: InChI=1S/C7H15N/c1-7-5-3-2-4-6-8-7/h7-8H,2-6H2,1H3
InchiKey: LGONGMXQDFYGKU-UHFFFAOYSA-N
Formula: C7H15N
SMILES: CC1CCCCCN1
Mol. weight [g/mol]: 113.20

Physical Properties

Property code	Value	Unit	Source
gf	108.12	kJ/mol	Joback Method
hf	-101.84	kJ/mol	Joback Method
hfus	13.21	kJ/mol	Joback Method
hvap	38.53	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.538		Crippen Method
mcvol	108.610	ml/mol	McGowan Method
pc	3740.80	kPa	Joback Method
rinpol	915.00		NIST Webbook
tb	431.93	K	Joback Method
tc	652.27	K	Joback Method
tf	277.54	K	Joback Method
vc	0.390	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.18	J/mol×K	431.93	Joback Method
cpg	231.85	J/mol×K	468.65	Joback Method
cpg	248.71	J/mol×K	505.38	Joback Method
cpg	264.75	J/mol×K	542.10	Joback Method
cpg	279.98	J/mol×K	578.82	Joback Method
cpg	294.40	J/mol×K	615.54	Joback Method
cpg	308.03	J/mol×K	652.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R405788&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