6H-1,4-diazepine, hexahydro-6-methyl-

Inchi: InChI=1S/C6H14N2/c1-6-4-7-2-3-8-5-6/h6-8H,2-5H2,1H3
InchiKey: VMJOIXFVKVPLRQ-UHFFFAOYSA-N
Formula: C6H14N2
SMILES: CC1CNCCNC1
Mol. weight [g/mol]: 114.19
CAS: 89582-17-2

Physical Properties

Property code	Value	Unit	Source
gf	187.41	kJ/mol	Joback Method
hf	-43.39	kJ/mol	Joback Method
hfus	20.21	kJ/mol	Joback Method
hvap	43.07	kJ/mol	Joback Method
log10ws	-0.37		Crippen Method
logp	-0.185		Crippen Method
mcvol	104.500	ml/mol	McGowan Method
pc	4362.63	kPa	Joback Method
tb	457.60	K	Joback Method
tc	688.59	K	Joback Method
tf	371.30	K	Joback Method
vc	0.370	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.63	J/mol×K	457.60	Joback Method
cpg	231.41	J/mol×K	496.10	Joback Method
cpg	247.44	J/mol×K	534.60	Joback Method
cpg	262.70	J/mol×K	573.09	Joback Method
cpg	277.19	J/mol×K	611.59	Joback Method
cpg	290.90	J/mol×K	650.09	Joback Method
cpg	303.81	J/mol×K	688.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C89582172&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume