7-Azanorbornene

Other names: 7-Azabicyclo(2,2,1)hept-2-ene
Inchi: InChI=1S/C6H9N/c1-2-6-4-3-5(1)7-6/h1-2,5-7H,3-4H2
InchiKey: DLAUQDHZCKKXBK-UHFFFAOYSA-N
Formula: C6H9N
SMILES: C1=CC2CCC1N2
Mol. weight [g/mol]: 95.14
CAS: 55590-24-4

Physical Properties

Property code	Value	Unit	Source
gf	226.71	kJ/mol	Joback Method
hf	67.86	kJ/mol	Joback Method
hfus	16.28	kJ/mol	Joback Method
hvap	36.00	kJ/mol	Joback Method
ie	8.30	eV	NIST Webbook
ie	8.75	eV	NIST Webbook
log10ws	-1.39		Crippen Method
logp	0.677		Crippen Method
mcvol	79.360	ml/mol	McGowan Method
pc	4769.39	kPa	Joback Method
tb	402.14	K	Joback Method
tc	618.90	K	Joback Method
tf	295.53	K	Joback Method
vc	0.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.10	J/mol×K	402.14	Joback Method
cpg	162.79	J/mol×K	438.27	Joback Method
cpg	175.54	J/mol×K	474.39	Joback Method
cpg	187.40	J/mol×K	510.52	Joback Method
cpg	198.44	J/mol×K	546.64	Joback Method
cpg	208.71	J/mol×K	582.77	Joback Method

cpg	218.26	J/mol×K	618.90	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55590244&Units=SI

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
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
tf:	Normal melting (fusion) point
vc:	Critical Volume