2,3-Diazabicyclo[2.2.2]oct-2-ene

Inchi: InChI=1S/C6H10N2/c1-2-6-4-3-5(1)7-8-6/h5-6H,1-4H2
InchiKey: JOHCCHGNXMXHPU-UHFFFAOYSA-N
Formula: C6H10N2
SMILES: C1CC2CCC1N=N2
Mol. weight [g/mol]: 110.16
CAS: 3310-62-1

Physical Properties

Property code	Value	Unit	Source
gf	360.46	kJ/mol	Joback Method
hf	165.83	kJ/mol	Joback Method
hfus	14.86	kJ/mol	Joback Method
hvap	41.83	kJ/mol	Joback Method
ie	7.79 ± 0.04	eV	NIST Webbook
ie	8.19	eV	NIST Webbook
ie	7.95	eV	NIST Webbook
log10ws	-1.61		Crippen Method
logp	1.763		Crippen Method
mcvol	89.340	ml/mol	McGowan Method
pc	4782.59	kPa	Joback Method
tb	465.26	K	Joback Method
tc	709.32	K	Joback Method
tf	330.06	K	Joback Method
vc	0.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.64	J/mol×K	465.26	Joback Method
cpg	233.02	J/mol×K	505.94	Joback Method
cpg	250.19	J/mol×K	546.61	Joback Method
cpg	266.20	J/mol×K	587.29	Joback Method
cpg	281.07	J/mol×K	627.97	Joback Method
cpg	294.83	J/mol×K	668.64	Joback Method

cpg	307.52	J/mol×K	709.32	Joback Method

Sources

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=C3310621&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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