Bicyclo[2.2.2]oct-5-en-2-one

Other names:	Bicyclo[2.2.2]octenone
	Bicyclo[2.2.2]oct-5-ene-2-one
Inchi:	InChI=1S/C8H10O/c9-8-5-6-1-3-7(8)4-2-6/h1,3,6-7H,2,4-5H2
InchiKey:	UJVGEBBKXJLFPB-UHFFFAOYSA-N
Formula:	C8H10O
SMILES:	O=C1CC2C=CC1CC2
Mol. weight [g/mol]:	122.16
CAS:	2220-40-8

Physical Properties

Property code	Value	Unit	Source
gf	21.15	kJ/mol	Joback Method
hf	-155.09	kJ/mol	Joback Method
hfus	9.28	kJ/mol	Joback Method
hvap	38.11	kJ/mol	Joback Method
ie	8.96 ± 0.05	eV	NIST Webbook
ie	8.73	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
log10ws	-1.61		Crippen Method
logp	1.542		Crippen Method
mcvol	99.130	ml/mol	McGowan Method
pc	3881.95	kPa	Joback Method
tb	471.44	K	Joback Method
tc	703.76	K	Joback Method
tf	277.74	K	Joback Method
vc	0.374	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.98	J/mol×K	471.44	Joback Method
cpg	232.91	J/mol×K	510.16	Joback Method
cpg	247.86	J/mol×K	548.88	Joback Method
cpg	261.87	J/mol×K	587.60	Joback Method

cpg	274.97	J/mol×K	626.32	Joback Method
cpg	287.21	J/mol×K	665.04	Joback Method
cpg	298.63	J/mol×K	703.76	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=C2220408&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