Bicyclo[2.2.1]hept-2-en-5-one

Other names:	Bicyclo(2.2.1)hept-5-en-2-one
	Dehydronorcamphor
	Norcamphor, dehydro-
	2-Norbornen-5-one
	2-Norbornenone
	5-Norbornen-2-one
Inchi:	InChI=1S/C7H8O/c8-7-4-5-1-2-6(7)3-5/h1-2,5-6H,3-4H2
InchiKey:	HUQXEIFQYCVOPD-UHFFFAOYSA-N
Formula:	C7H8O
SMILES:	O=C1CC2C=CC1C2
Mol. weight [g/mol]:	108.14
CAS:	694-98-4

Physical Properties

Property code	Value	Unit	Source
affp	845.30	kJ/mol	NIST Webbook
basg	813.40	kJ/mol	NIST Webbook
gf	24.83	kJ/mol	Joback Method
hf	-128.29	kJ/mol	Joback Method
hfus	8.79	kJ/mol	Joback Method
hvap	35.71	kJ/mol	Joback Method
ie	8.90 ± 0.02	eV	NIST Webbook
ie	8.86	eV	NIST Webbook
log10ws	-1.19		Crippen Method
logp	1.151		Crippen Method
mcvol	85.040	ml/mol	McGowan Method
pc	4249.61	kPa	Joback Method
rinpol	931.00		NIST Webbook
tb	444.29	K	Joback Method
tc	671.01	K	Joback Method
tf	269.99	K	Joback Method
vc	0.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.45	J/mol×K	444.29	Joback Method
cpg	190.19	J/mol×K	482.08	Joback Method
cpg	203.08	J/mol×K	519.86	Joback Method
cpg	215.13	J/mol×K	557.65	Joback Method
cpg	226.41	J/mol×K	595.44	Joback Method
cpg	236.95	J/mol×K	633.22	Joback Method
cpg	246.79	J/mol×K	671.01	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=C694984&Units=SI

Legend

affp: Proton affinity
basg: Gas basicity
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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume