Norbornadieone

Other names:	Bicyclo[2.2.1]heptan-7-one
	Norbornan-7-one
Inchi:	InChI=1S/C7H10O/c8-7-5-1-2-6(7)4-3-5/h5-6H,1-4H2
InchiKey:	ZESXVLLAIXOYKB-UHFFFAOYSA-N
Formula:	C7H10O
SMILES:	O=C1C2CCC1CC2
Mol. weight [g/mol]:	110.15
CAS:	10218-02-7

Physical Properties

Property code	Value	Unit	Source
affp	832.10	kJ/mol	NIST Webbook
basg	802.40	kJ/mol	NIST Webbook
chs	-4002.40 ± 2.30	kJ/mol	NIST Webbook
gf	-5.13	kJ/mol	Joback Method
hf	-134.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-181.30 ± 2.30	kJ/mol	NIST Webbook
hfus	7.57	kJ/mol	Joback Method
hsub	47.30 ± 2.20	kJ/mol	NIST Webbook
hsub	47.00 ± 2.00	kJ/mol	NIST Webbook
hvap	46.65	kJ/mol	NIST Webbook
ie	9.01 ± 0.02	eV	NIST Webbook
ie	9.06	eV	NIST Webbook
log10ws	-1.34		Crippen Method
logp	1.375		Crippen Method
mcvol	89.340	ml/mol	McGowan Method
pc	4056.96	kPa	Joback Method
tb	445.13	K	Joback Method
tc	669.43	K	Joback Method
tf	269.23	K	Joback Method
vc	0.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.02	J/mol×K	445.13	Joback Method
cpg	206.16	J/mol×K	482.51	Joback Method
cpg	220.39	J/mol×K	519.90	Joback Method
cpg	233.77	J/mol×K	557.28	Joback Method
cpg	246.33	J/mol×K	594.66	Joback Method
cpg	258.10	J/mol×K	632.05	Joback Method
cpg	269.14	J/mol×K	669.43	Joback Method
hvapt	47.90	kJ/mol	335.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10218027&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

Legend

affp: Proton affinity
basg: Gas basicity
chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsub: Enthalpy of sublimation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
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