7-Oxabicyclo[2.2.1]heptane

Other names:	7-Oxanorbornane
	Cyclohexane, 1,4-epoxy-
	Cyclohexane, 3,6-endoxo-
	1,4-Epoxycyclohexane
	1,4-Oxycyclohexane
	3,6-Endooxycyclohexane
	3,6-Endoxocyclohexane
	Bicyclo[2.2.1]heptane, 7-oxa-
Inchi:	InChI=1S/C6H10O/c1-2-6-4-3-5(1)7-6/h5-6H,1-4H2
InchiKey:	YPWFNLSXQIGJCK-UHFFFAOYSA-N
Formula:	C6H10O
SMILES:	C1CC2CCC1O2
Mol. weight [g/mol]:	98.14
CAS:	279-49-2

Physical Properties

Property code	Value	Unit	Source
affp	844.20	kJ/mol	NIST Webbook
basg	816.80	kJ/mol	NIST Webbook
chl	-3566.30 ± 1.50	kJ/mol	NIST Webbook
chl	-3566.30 ± 1.50	kJ/mol	NIST Webbook
gf	22.92	kJ/mol	Joback Method
hf	-159.73	kJ/mol	Joback Method
hfl	-223.90 ± 2.00	kJ/mol	NIST Webbook
hfus	13.44	kJ/mol	Joback Method
hvap	33.46	kJ/mol	Joback Method
ie	9.57 ± 0.02	eV	NIST Webbook
log10ws	-1.43		Crippen Method
logp	1.328		Crippen Method
mcvol	79.550	ml/mol	McGowan Method
pc	4339.67	kPa	Joback Method
tb	381.38	K	Joback Method
tc	586.65	K	Joback Method
tf	216.31	K	Joback Method
vc	0.298	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	151.20	J/mol×K	381.38	Joback Method
cpg	165.70	J/mol×K	415.59	Joback Method
cpg	179.24	J/mol×K	449.80	Joback Method
cpg	191.89	J/mol×K	484.02	Joback Method
cpg	203.68	J/mol×K	518.23	Joback Method
cpg	214.68	J/mol×K	552.44	Joback Method
cpg	224.93	J/mol×K	586.65	Joback Method
dvisc	0.0009627	Pa×s	216.31	Joback Method
dvisc	0.0008301	Pa×s	243.82	Joback Method
dvisc	0.0007377	Pa×s	271.33	Joback Method
dvisc	0.0006699	Pa×s	298.85	Joback Method
dvisc	0.0006183	Pa×s	326.36	Joback Method
dvisc	0.0005779	Pa×s	353.87	Joback Method
dvisc	0.0005454	Pa×s	381.38	Joback Method
hfust	0.71	kJ/mol	244.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	392.20	K	95.10	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C279492&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume