7-Oxabicyclo[4.1.0]heptane

Other names:	1,2-cyclohexene oxide 1,2-epoxycyclohexane 2,3-tetramethyleneoxirane Bicyclo[4.1.0]heptane, 7-oxa- CCHO Cyclohexene 1-oxide NSC 128074 cyclohexane, 1,2-epoxy- cyclohexene epoxide cyclohexene oxide cyclohexylene oxide tetramethyleneoxirane
Inchi:	InChI=1S/C6H10O/c1-2-4-6-5(3-1)7-6/h5-6H,1-4H2
InchiKey:	ZWAJLVLEBYIOTI-UHFFFAOYSA-N
Formula:	C6H10O
SMILES:	C1CCC2OC2C1
Mol. weight [g/mol]:	98.14
CAS:	286-20-4

Physical Properties

Property code	Value	Unit	Source
affp	848.10	kJ/mol	NIST Webbook
basg	815.60	kJ/mol	NIST Webbook
chl	-3624.20 ± 1.00	kJ/mol	NIST Webbook
chl	-3624.90 ± 0.60	kJ/mol	NIST Webbook
gf	22.92	kJ/mol	Joback Method
hf	-122.20 ± 2.20	kJ/mol	NIST Webbook
hf	-125.50 ± 1.10	kJ/mol	NIST Webbook
hfl	-165.30 ± 1.00	kJ/mol	NIST Webbook
hfl	-166.00 ± 1.10	kJ/mol	NIST Webbook
hfus	13.44	kJ/mol	Joback Method
hvap	40.50 ± 0.20	kJ/mol	NIST Webbook
hvap	43.10	kJ/mol	NIST Webbook
hvap	40.50	kJ/mol	NIST Webbook
hvap	43.20 ± 2.00	kJ/mol	NIST Webbook
ie	9.82	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
ripol	1158.00		NIST Webbook
ripol	1152.00		NIST Webbook
ripol	1158.00		NIST Webbook
sl	221.98	J/mol×K	NIST Webbook
tb	402.50 ± 0.50	K	NIST Webbook
tb	404.87	K	Measurement and Modeling of the High-Pressure Phase Behavior of the Binary System Carbon Dioxide + 1,2-Epoxycyclohexane
tb	402.70	K	NIST Webbook
tb	404.70	K	NIST Webbook
tc	586.65	K	Joback Method
tf	216.31	K	Joback Method
tt	238.14 ± 0.01	K	NIST Webbook
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
cpl	166.12	J/mol×K	300.00	NIST Webbook
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	1.06	kJ/mol	238.10	NIST Webbook
hfust	9.54	kJ/mol	193.10	NIST Webbook
hfust	1.06	kJ/mol	155.00	NIST Webbook

pvap	25.50	kPa	360.91	Measurement and Modeling of the High-Pressure Phase Behavior of the Binary System Carbon Dioxide + 1,2-Epoxycyclohexane
pvap	25.80	kPa	361.13	Measurement and Modeling of the High-Pressure Phase Behavior of the Binary System Carbon Dioxide + 1,2-Epoxycyclohexane
pvap	52.40	kPa	382.47	Measurement and Modeling of the High-Pressure Phase Behavior of the Binary System Carbon Dioxide + 1,2-Epoxycyclohexane
pvap	53.60	kPa	383.09	Measurement and Modeling of the High-Pressure Phase Behavior of the Binary System Carbon Dioxide + 1,2-Epoxycyclohexane
pvap	101.30	kPa	404.87	Measurement and Modeling of the High-Pressure Phase Behavior of the Binary System Carbon Dioxide + 1,2-Epoxycyclohexane
pvap	103.80	kPa	405.48	Measurement and Modeling of the High-Pressure Phase Behavior of the Binary System Carbon Dioxide + 1,2-Epoxycyclohexane
pvap	167.00	kPa	423.87	Measurement and Modeling of the High-Pressure Phase Behavior of the Binary System Carbon Dioxide + 1,2-Epoxycyclohexane

pvap	268.00	kPa	443.95	Measurement and Modeling of the High-Pressure Phase Behavior of the Binary System Carbon Dioxide + 1,2-Epoxycyclohexane
pvap	333.00	kPa	453.99	Measurement and Modeling of the High-Pressure Phase Behavior of the Binary System Carbon Dioxide + 1,2-Epoxycyclohexane
pvap	409.00	kPa	463.99	Measurement and Modeling of the High-Pressure Phase Behavior of the Binary System Carbon Dioxide + 1,2-Epoxycyclohexane
pvap	497.00	kPa	474.03	Measurement and Modeling of the High-Pressure Phase Behavior of the Binary System Carbon Dioxide + 1,2-Epoxycyclohexane
sfust	49.38	J/mol×K	193.10	NIST Webbook
sfust	4.47	J/mol×K	238.10	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Measurement and Modeling of the High-Pressure Phase Behavior of the Binary System Carbon Dioxide + 1,2-Epoxycyclohexane:	https://www.doi.org/10.1021/je050156k
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=C286204&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
pvap:	Vapor pressure
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume