

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	-166.00 ± 1.10	kJ/mol	NIST Webbook
hfl	-165.30 ± 1.00	kJ/mol	NIST Webbook
hfus	13.44	kJ/mol	Joback Method
hvap	43.10	kJ/mol	NIST Webbook
hvap	43.20 ± 2.00	kJ/mol	NIST Webbook
hvap	40.50 ± 0.20	kJ/mol	NIST Webbook
hvap	40.50	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	1158.00		NIST Webbook
ripol	1152.00		NIST Webbook
sl	221.98	J/mol×K	NIST Webbook
tb	402.50 ± 0.50	K	NIST Webbook
tb	404.70	K	NIST Webbook
tb	402.70	K	NIST Webbook
tb	404.87	K	Measurement and Modeling of the High-Pressure Phase Behavior of the Binary System Carbon Dioxide + 1,2-Epoxyhexane
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	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
cpg	151.20	J/mol×K	381.38	Joback Method
cpl	166.12	J/mol×K	300.00	NIST Webbook
dvisc	0.0008301	Paxs	243.82	Joback Method
dvisc	0.0007377	Paxs	271.33	Joback Method
dvisc	0.0006699	Paxs	298.85	Joback Method
dvisc	0.0006183	Paxs	326.36	Joback Method
dvisc	0.0005779	Paxs	353.87	Joback Method
dvisc	0.0005454	Paxs	381.38	Joback Method
dvisc	0.0009627	Paxs	216.31	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-Epoxyhexane
pvap	497.00	kPa	474.03	Measurement and Modeling of the High-Pressure Phase Behavior of the Binary System Carbon Dioxide + 1,2-Epoxyhexane
pvap	409.00	kPa	463.99	Measurement and Modeling of the High-Pressure Phase Behavior of the Binary System Carbon Dioxide + 1,2-Epoxyhexane
pvap	333.00	kPa	453.99	Measurement and Modeling of the High-Pressure Phase Behavior of the Binary System Carbon Dioxide + 1,2-Epoxyhexane
pvap	268.00	kPa	443.95	Measurement and Modeling of the High-Pressure Phase Behavior of the Binary System Carbon Dioxide + 1,2-Epoxyhexane
pvap	167.00	kPa	423.87	Measurement and Modeling of the High-Pressure Phase Behavior of the Binary System Carbon Dioxide + 1,2-Epoxyhexane
pvap	103.80	kPa	405.48	Measurement and Modeling of the High-Pressure Phase Behavior of the Binary System Carbon Dioxide + 1,2-Epoxyhexane

pvap	101.30	kPa	404.87	Measurement and Modeling of the High-Pressure Phase Behavior of the Binary System Carbon Dioxide + 1,2-Epoxyhexane
pvap	53.60	kPa	383.09	Measurement and Modeling of the High-Pressure Phase Behavior of the Binary System Carbon Dioxide + 1,2-Epoxyhexane
pvap	52.40	kPa	382.47	Measurement and Modeling of the High-Pressure Phase Behavior of the Binary System Carbon Dioxide + 1,2-Epoxyhexane
pvap	25.80	kPa	361.13	Measurement and Modeling of the High-Pressure Phase Behavior of the Binary System Carbon Dioxide + 1,2-Epoxyhexane
sfust	49.38	J/mol·K	193.10	NIST Webbook
sfust	4.47	J/mol·K	238.10	NIST Webbook

Sources

Measurement and Modeling of the High-Pressure Phase Behavior of the Binary System Carbon Dioxide + 1,2-Epoxyhexane: McGowan Method:

<https://www.doi.org/10.1021/je050156k>

https://en.wikipedia.org/wiki/Joback_method

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C286204&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

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

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