Cycloheptanone

Other names:	KETOCYCLOHEPTANE
	Ketoheptamethylene
	SUBERONE
	Suberon
Inchi:	InChI=1S/C7H12O/c8-7-5-3-1-2-4-6-7/h1-6H2
InchiKey:	CGZZMOTZOONQIA-UHFFFAOYSA-N
Formula:	C7H12O
SMILES:	O=C1CCCCCC1
Mol. weight [g/mol]:	112.17
CAS:	502-42-1

Physical Properties

Property code	Value	Unit	Source
affp	845.60	kJ/mol	NIST Webbook
affp	846.30 ± 0.20	kJ/mol	NIST Webbook
basg	815.90	kJ/mol	NIST Webbook
chl	-4172.00	kJ/mol	NIST Webbook
chl	-4203.20	kJ/mol	NIST Webbook
chl	-4170.20 ± 1.30	kJ/mol	NIST Webbook
chl	-4172.00 ± 1.00	kJ/mol	NIST Webbook
gf	-94.47	kJ/mol	Joback Method
hf	-248.00 ± 1.30	kJ/mol	NIST Webbook
hf	-247.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-297.60 ± 1.10	kJ/mol	NIST Webbook
hfl	-299.00 ± 1.00	kJ/mol	NIST Webbook
hfus	2.06	kJ/mol	Joback Method
hvap	51.90	kJ/mol	NIST Webbook
hvap	50.70	kJ/mol	NIST Webbook
hvap	49.54 ± 0.63	kJ/mol	NIST Webbook
hvap	49.50 ± 0.60	kJ/mol	NIST Webbook
hvap	52.00 ± 1.00	kJ/mol	NIST Webbook
hvap	50.60	kJ/mol	NIST Webbook
ie	9.17 ± 0.02	eV	NIST Webbook
ie	9.14	eV	NIST Webbook
ie	9.49 ± 0.01	eV	NIST Webbook
log10ws	-1.93		Crippen Method
logp	1.910		Crippen Method

mcvol	100.200	ml/mol	McGowan Method
pc	3945.61	kPa	Joback Method
rinpol	999.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	981.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	987.00		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	992.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	979.00		NIST Webbook
rinpol	992.00		NIST Webbook
rinpol	1015.50		NIST Webbook
rinpol	1005.10		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	1009.00		NIST Webbook
rinpol	989.00		NIST Webbook
ripol	1495.00		NIST Webbook
ripol	1495.00		NIST Webbook
tb	453.15 ± 3.00	K	NIST Webbook
tb	451.70	K	NIST Webbook
tb	452.95 ± 0.60	K	NIST Webbook
tc	689.15	K	Joback Method
tf	244.97	K	Joback Method
vc	0.360	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	202.51	J/mol×K	455.87	Joback Method
cpg	219.00	J/mol×K	494.75	Joback Method
cpg	234.73	J/mol×K	533.63	Joback Method
cpg	249.68	J/mol×K	572.51	Joback Method
cpg	263.85	J/mol×K	611.39	Joback Method
cpg	277.23	J/mol×K	650.27	Joback Method
cpg	289.79	J/mol×K	689.15	Joback Method
hfust	1.39	kJ/mol	259.30	NIST Webbook
hfust	12.40	kJ/mol	227.00	NIST Webbook
hfust	0.43	kJ/mol	232.60	NIST Webbook

hfust	1.39	kJ/mol	259.30	NIST Webbook
hvapt	48.50	kJ/mol	383.00	NIST Webbook
hvapt	44.80	kJ/mol	419.00	NIST Webbook
rhol	950.20	kg/m3	298.15	Excess molar enthalpies for binary mixtures of cyclopentanone, cyclohexanone, or cycloheptanone with n-nonane at T = 298.15 K and atmospheric pressure
rhol	951.85	kg/m3	293.15	Thermodynamic Studies of Molecular Interactions in Mixtures Containing Tetrahydropyran, 1,4-dioxane and Cyclic ketones
rhol	947.62	kg/m3	298.15	Thermodynamic Studies of Molecular Interactions in Mixtures Containing Tetrahydropyran, 1,4-dioxane and Cyclic ketones
rhol	943.38	kg/m3	303.15	Thermodynamic Studies of Molecular Interactions in Mixtures Containing Tetrahydropyran, 1,4-dioxane and Cyclic ketones
rhol	939.14	kg/m3	308.15	Thermodynamic Studies of Molecular Interactions in Mixtures Containing Tetrahydropyran, 1,4-dioxane and Cyclic ketones
sfust	54.60	J/mol×K	227.00	NIST Webbook
sfust	1.80	J/mol×K	232.60	NIST Webbook
sfust	5.40	J/mol×K	259.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39934e+01
Coeff. B	-3.54832e+03
Coeff. C	-7.31660e+01
Temperature range (K), min.	332.06
Temperature range (K), max.	481.87

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.20417e+01
Coeff. B	-9.03252e+03
Coeff. C	-1.12400e+01
Coeff. D	6.06481e-06
Temperature range (K), min.	373.15
Temperature range (K), max.	464.15

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1228
Excess molar volumes and excess isentropic compressibilities of mixtures containing lactam, cyclic ethers and cyclic alkanones:	https://www.doi.org/10.1016/j.jct.2018.05.012
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Partial molar volumes of organic solutes in water. XXIII. Cyclic ketones at T = (298 to 373) K and pressures up to 30 MPa:	https://www.doi.org/10.1016/j.jct.2011.02.010
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Odd Even Effects in the Static Dielectric Permittivity of a Homologous Series of Liquid Cycloalkanones, (CH2)n-1C-O, n = 4 to 8:	https://www.doi.org/10.1021/je200682t
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Thermodynamic Studies of Molecular Interactions in Mixtures Containing Tetrahydropyran, 1,4-dioxane and Cyclic ketones:	https://www.doi.org/10.1021/acs.jced.6b00606
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1228.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C502421&Units=SI
Excess molar enthalpies for binary mixtures of cyclopentanone, cyclohexanone, or cycloheptanone with n-nonane at T = 298.15 K and atmospheric pressure:	https://www.doi.org/10.1016/j.jct.2014.03.007
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
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
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
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume