Cyclobutanone

Inchi: InChI=1S/C4H6O/c5-4-2-1-3-4/h1-3H2
InchiKey: SHQSVMDWKBRBGB-UHFFFAOYSA-N
Formula: C4H6O
SMILES: O=C1CCC1
Mol. weight [g/mol]: 70.09
CAS: 1191-95-3

Physical Properties

Property code	Value	Unit	Source
affp	802.50	kJ/mol	NIST Webbook
basg	772.70	kJ/mol	NIST Webbook
chl	-2292.10 ± 1.20	kJ/mol	NIST Webbook
chl	-2300.70 ± 0.63	kJ/mol	NIST Webbook
ea	9.99e-04	eV	NIST Webbook
gf	-83.43	kJ/mol	Joback Method
hf	-91.60	kJ/mol	NIST Webbook
hf	-101.00 ± 1.00	kJ/mol	NIST Webbook
hfl	-139.50 ± 1.20	kJ/mol	NIST Webbook
hfl	-131.00	kJ/mol	NIST Webbook
hfus	0.59	kJ/mol	Joback Method
hvap	38.20 ± 0.40	kJ/mol	NIST Webbook
hvap	38.20 ± 0.42	kJ/mol	NIST Webbook
hvap	38.30	kJ/mol	NIST Webbook
hvap	38.40	kJ/mol	NIST Webbook
ie	9.35	eV	NIST Webbook
ie	9.40 ± 0.10	eV	NIST Webbook
ie	9.35	eV	NIST Webbook
ie	9.60 ± 0.10	eV	NIST Webbook
ie	9.61 ± 0.02	eV	NIST Webbook
log10ws	-0.67		Crippen Method
logp	0.739		Crippen Method
mcvol	57.930	ml/mol	McGowan Method
pc	5258.62	kPa	Joback Method
rinpol	633.00		NIST Webbook
rinpol	639.00		NIST Webbook
rinpol	645.00		NIST Webbook
rinpol	641.00		NIST Webbook

rinpol	641.00		NIST Webbook
rinpol	639.00		NIST Webbook
rinpol	642.00		NIST Webbook
rinpol	647.00		NIST Webbook
rinpol	642.00		NIST Webbook
rinpol	647.00		NIST Webbook
tb	372.05	K	KDB
tb	372.20	K	NIST Webbook
tb	372.90 ± 0.50	K	NIST Webbook
tb	372.20 ± 4.00	K	NIST Webbook
tb	1171.15 ± 1.50	K	NIST Webbook
tc	587.84	K	Joback Method
tf	221.72	K	Joback Method
vc	0.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	93.90	J/mol×K	374.42	Joback Method
cpg	102.89	J/mol×K	409.99	Joback Method
cpg	111.48	J/mol×K	445.56	Joback Method
cpg	119.70	J/mol×K	481.13	Joback Method
cpg	127.54	J/mol×K	516.70	Joback Method
cpg	135.01	J/mol×K	552.27	Joback Method
cpg	142.11	J/mol×K	587.84	Joback Method
hfust	10.80	kJ/mol	220.50	NIST Webbook
hfust	10.80	kJ/mol	220.50	NIST Webbook
hvapt	37.70	kJ/mol	322.50	NIST Webbook
hvapt	36.30	kJ/mol	348.50	NIST Webbook
hvapt	38.50	kJ/mol	273.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46360e+01
Coeff. B	-3.24879e+03

Coeff. C	-4.78950e+01
Temperature range (K), min.	274.32
Temperature range (K), max.	396.31

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.68593e+01
Coeff. B	-7.17622e+03
Coeff. C	-1.08793e+01
Coeff. D	1.04245e-05
Temperature range (K), min.	249.15
Temperature range (K), max.	380.15

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1219
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1191953&Units=SI
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1219
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
ea:	Electron affinity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume