Cyclooctanone

Inchi: InChI=1S/C8H14O/c9-8-6-4-2-1-3-5-7-8/h1-7H2
InchiKey: IIRFCWANHMSDCG-UHFFFAOYSA-N
Formula: C8H14O
SMILES: O=C1CCCCCCC1
Mol. weight [g/mol]: 126.20
CAS: 502-49-8

Physical Properties

Property code	Value	Unit	Source
affp	849.40	kJ/mol	NIST Webbook
basg	819.60	kJ/mol	NIST Webbook
chs	-4822.90 ± 5.00	kJ/mol	NIST Webbook
chs	-4825.60 ± 1.60	kJ/mol	NIST Webbook
gf	-98.15	kJ/mol	Joback Method
hf	-272.00 ± 5.40	kJ/mol	NIST Webbook
hf	-272.20 ± 1.80	kJ/mol	NIST Webbook
hfl	-326.00 ± 5.00	kJ/mol	NIST Webbook
hfs	-322.30 ± 1.60	kJ/mol	NIST Webbook
hfus	2.55	kJ/mol	Joback Method
hvap	54.40	kJ/mol	NIST Webbook
hvap	53.60	kJ/mol	NIST Webbook
hvap	54.20	kJ/mol	NIST Webbook
hvap	54.00 ± 2.00	kJ/mol	NIST Webbook
hvap	48.50 ± 0.60	kJ/mol	NIST Webbook
ie	9.08	eV	NIST Webbook
ie	9.28	eV	NIST Webbook
ie	9.28	eV	NIST Webbook
ie	9.09 ± 0.02	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
log10ws	-2.35		Crippen Method
logp	2.300		Crippen Method
mcvol	114.290	ml/mol	McGowan Method
pc	3615.89	kPa	Joback Method
rinpol	1096.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1115.00		NIST Webbook
rinpol	1104.00		NIST Webbook

rinpol	1093.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1115.00		NIST Webbook
tb	469.15 ± 3.00	K	NIST Webbook
tb	478.70 ± 0.50	K	NIST Webbook
tb	469.20	K	NIST Webbook
tc	721.71	K	Joback Method
tf	298.65 ± 2.00	K	NIST Webbook
tf	317.40 ± 0.10	K	NIST Webbook
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.21	J/mol×K	602.36	Joback Method
cpg	315.24	J/mol×K	642.15	Joback Method
cpg	330.30	J/mol×K	681.93	Joback Method
cpg	245.43	J/mol×K	483.02	Joback Method
cpg	264.28	J/mol×K	522.80	Joback Method
cpg	282.21	J/mol×K	562.58	Joback Method
cpg	344.35	J/mol×K	721.71	Joback Method
hfust	2.51	kJ/mol	174.00	NIST Webbook
hfust	13.80	kJ/mol	226.80	NIST Webbook
hfust	2.87	kJ/mol	318.70	NIST Webbook
hvapt	46.80	kJ/mol	439.00	NIST Webbook
hvapt	47.30	kJ/mol	363.00	NIST Webbook
sfust	9.00	J/mol×K	318.70	NIST Webbook
sfust	60.80	J/mol×K	226.80	NIST Webbook
sfust	14.40	J/mol×K	174.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.89566e+01
Coeff. B	-9.79197e+03

Coeff. C	-1.21808e+01
Coeff. D	6.02535e-06
Temperature range (K), min.	394.15
Temperature range (K), max.	483.15

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1229
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1229.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C502498&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid 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
hfs:	Solid 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
sfust:	Entropy of fusion at a given temperature

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume