2-Cyclopenten-1-one

Other names:	1-cyclopenten-3-one
	2-Cyclopentenone
	2-Cyclopentenone-1
	3-Cyclopenten-2-one
	Cyclopenten-3-one
	Cyclopentenone
	cyclopenten-2-one
Inchi:	InChI=1S/C5H6O/c6-5-3-1-2-4-5/h1,3H,2,4H2
InchiKey:	BZKFMUIJRXWWQK-UHFFFAOYSA-N
Formula:	C5H6O
SMILES:	O=C1C=CCC1
Mol. weight [g/mol]:	82.10
CAS:	930-30-3

Physical Properties

Property code	Value	Unit	Source
gf	-57.15	kJ/mol	Joback Method
hf	-145.63	kJ/mol	Joback Method
hfus	2.30	kJ/mol	Joback Method
hvap	31.83	kJ/mol	Joback Method
ie	9.34 ± 0.02	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
ie	8.47 ± 0.05	eV	NIST Webbook
ie	9.35	eV	NIST Webbook
log10ws	-0.94		Crippen Method
logp	0.905		Crippen Method
mcvol	67.720	ml/mol	McGowan Method
pc	5001.51	kPa	Joback Method
rinpol	802.00		NIST Webbook
rinpol	781.00		NIST Webbook
rinpol	802.00		NIST Webbook
rinpol	799.00		NIST Webbook
rinpol	834.90		NIST Webbook
rinpol	799.00		NIST Webbook
rinpol	793.00		NIST Webbook
rinpol	793.00		NIST Webbook
rinpol	834.90		NIST Webbook

ripol	1341.00		NIST Webbook
ripol	1344.00		NIST Webbook
ripol	1344.00		NIST Webbook
ripol	1309.00		NIST Webbook
ripol	1313.00		NIST Webbook
ripol	1335.00		NIST Webbook
ripol	1372.00		NIST Webbook
ripol	1383.00		NIST Webbook
ripol	1372.00		NIST Webbook
ripol	1313.00		NIST Webbook
ripol	1316.00		NIST Webbook
ripol	1385.00		NIST Webbook
ripol	1385.00		NIST Webbook
ripol	1349.00		NIST Webbook
ripol	1345.00		NIST Webbook
ripol	1347.00		NIST Webbook
ripol	1342.00		NIST Webbook
ripol	1343.00		NIST Webbook
ripol	1344.00		NIST Webbook
ripol	1343.00		NIST Webbook
tb	409.20	K	NIST Webbook
tc	623.87	K	Joback Method
tf	230.23	K	Joback Method
vc	0.251	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	113.99	J/mol×K	400.73	Joback Method
cpg	124.04	J/mol×K	437.92	Joback Method
cpg	133.64	J/mol×K	475.11	Joback Method
cpg	142.78	J/mol×K	512.30	Joback Method
cpg	151.48	J/mol×K	549.49	Joback Method
cpg	159.72	J/mol×K	586.68	Joback Method
cpg	167.52	J/mol×K	623.87	Joback Method
hvapt	52.40	kJ/mol	298.15	Energetic vs structural study of two biomass degradation derivatives: 2-Cyclopentenone and 3-methyl-2-cyclopentenone

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	337.70	K	2.50	NIST Webbook
tbrp	313.20	K	1.60	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C930303&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Energetic vs structural study of two biomass degradation derivatives: 2-Cyclopentenone and 3-methyl-2-cyclopentenone:	https://www.doi.org/10.1016/j.jct.2019.01.012
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume