

1-Propanone, 1-(1-cyclohexen-1-yl)-

Other names:	1-(1-cyclohexen-1-yl)-1-propanone
Inchi:	InChI=1S/C9H14O/c1-2-9(10)8-6-4-3-5-7-8/h6H,2-5,7H2,1H3
InchiKey:	UZKJRXTYIKFJQV-UHFFFAOYSA-N
Formula:	C9H14O
SMILES:	CCC(=O)C1=CCCCC1
Mol. weight [g/mol]:	138.21
CAS:	1655-03-4

Physical Properties

Property code	Value	Unit	Source
gf	-51.53	kJ/mol	Joback Method
hf	-220.70	kJ/mol	Joback Method
hfus	12.26	kJ/mol	Joback Method
hvap	44.07	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.466		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
ripol	1620.00		NIST Webbook
tb	487.55	K	Joback Method
tc	701.51	K	Joback Method
tf	266.02	K	Joback Method
vc	0.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.11	J/molxK	487.55	Joback Method
cpg	281.60	J/molxK	523.21	Joback Method
cpg	296.23	J/molxK	558.87	Joback Method
cpg	310.02	J/molxK	594.53	Joback Method
cpg	323.00	J/molxK	630.19	Joback Method
cpg	335.19	J/molxK	665.85	Joback Method
cpg	346.64	J/molxK	701.51	Joback Method

dvisc	0.0045184	Paxs	266.02	Joback Method
dvisc	0.0021422	Paxs	302.94	Joback Method
dvisc	0.0011944	Paxs	339.86	Joback Method
dvisc	0.0007468	Paxs	376.78	Joback Method
dvisc	0.0005077	Paxs	413.71	Joback Method
dvisc	0.0003677	Paxs	450.63	Joback Method
dvisc	0.0002796	Paxs	487.55	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1655034&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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