

Ethanone, 1-(2-methyl-1-cyclopenten-1-yl)-

Other names:	Ketone, methyl 2-methyl-1-cyclopenten-1-yl 1-Acetyl-2-methylcyclopentene 1-Acetyl-2-methyl-1-cyclopentene
Inchi:	InChI=1S/C8H12O/c1-6-4-3-5-8(6)7(2)9/h3-5H2,1-2H3
InchiKey:	HDURLXYBKGWETC-UHFFFAOYSA-N
Formula:	C8H12O
SMILES:	CC(=O)C1=C(C)CCC1
Mol. weight [g/mol]:	124.18
CAS:	3168-90-9

Physical Properties

Property code	Value	Unit	Source
gf	-57.48	kJ/mol	Joback Method
hf	-205.37	kJ/mol	Joback Method
hfus	11.38	kJ/mol	Joback Method
hvap	42.33	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	2.076		Crippen Method
mcvol	109.990	ml/mol	McGowan Method
pc	3443.98	kPa	Joback Method
ripol	1504.00		NIST Webbook
ripol	1504.00		NIST Webbook
tb	462.70	K	NIST Webbook
tc	675.58	K	Joback Method
tf	270.79	K	Joback Method
vc	0.417	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.49	J/mol×K	465.38	Joback Method
cpg	283.12	J/mol×K	640.55	Joback Method
cpg	272.69	J/mol×K	605.52	Joback Method
cpg	261.63	J/mol×K	570.48	Joback Method

cpg	249.93	J/molxK	535.45	Joback Method
cpg	237.56	J/molxK	500.41	Joback Method
cpg	292.97	J/molxK	675.58	Joback Method
dvisc	0.0003325	Paxs	465.38	Joback Method
dvisc	0.0004080	Paxs	432.95	Joback Method
dvisc	0.0005174	Paxs	400.52	Joback Method
dvisc	0.0006841	Paxs	368.09	Joback Method
dvisc	0.0009549	Paxs	335.65	Joback Method
dvisc	0.0014313	Paxs	303.22	Joback Method
dvisc	0.0023639	Paxs	270.79	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C3168909&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
mcvol:	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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