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	m3/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/mol×K	535.45	Joback Method
cpg	237.56	J/mol×K	500.41	Joback Method
cpg	292.97	J/mol×K	675.58	Joback Method
dvisc	0.0003325	Pa×s	465.38	Joback Method
dvisc	0.0004080	Pa×s	432.95	Joback Method
dvisc	0.0005174	Pa×s	400.52	Joback Method
dvisc	0.0006841	Pa×s	368.09	Joback Method
dvisc	0.0009549	Pa×s	335.65	Joback Method
dvisc	0.0014313	Pa×s	303.22	Joback Method
dvisc	0.0023639	Pa×s	270.79	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=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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