

Ethanone, 1-(2-methylcyclopropyl)-

Other names:	Ketone, methyl 2-methylcyclopropyl Methyl 2-methylcyclopropyl ketone 2-Methylcyclopropyl methyl ketone
Inchi:	InChI=1S/C6H10O/c1-4-3-6(4)5(2)7/h4,6H,3H2,1-2H3
InchiKey:	CSEAGYCTZLEZON-UHFFFAOYSA-N
Formula:	C6H10O
SMILES:	CC(=O)C1CC1C
Mol. weight [g/mol]:	98.14
CAS:	930-56-3

Physical Properties

Property code	Value	Unit	Source
gf	-76.24	kJ/mol	Joback Method
hf	-227.29	kJ/mol	Joback Method
hfus	12.10	kJ/mol	Joback Method
hvap	35.30	kJ/mol	Joback Method
ie	9.38	eV	NIST Webbook
log10ws	-1.03		Crippen Method
logp	1.231		Crippen Method
mcvol	86.110	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
tb	392.62	K	Joback Method
tc	585.16	K	Joback Method
tf	221.01	K	Joback Method
vc	0.334	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	161.87	J/mol×K	392.62	Joback Method
cpg	173.58	J/mol×K	424.71	Joback Method
cpg	184.68	J/mol×K	456.80	Joback Method
cpg	195.20	J/mol×K	488.89	Joback Method
cpg	205.17	J/mol×K	520.98	Joback Method

cpg	214.61	J/mol×K	553.07	Joback Method
cpg	223.54	J/mol×K	585.16	Joback Method
dvisc	0.0008422	Pa×s	221.01	Joback Method
dvisc	0.0006995	Pa×s	249.61	Joback Method
dvisc	0.0006036	Pa×s	278.21	Joback Method
dvisc	0.0005354	Pa×s	306.81	Joback Method
dvisc	0.0004847	Pa×s	335.42	Joback Method
dvisc	0.0004457	Pa×s	364.02	Joback Method
dvisc	0.0004149	Pa×s	392.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C930563&Units=SI
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

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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