Ethanone, 1-cyclobutyl-

Other names:	Ketone, cyclobutyl methyl
	Acetylcyclobutane
	Cyclobutane, acetyl-
	Cyclobutyl methyl ketone
	Methyl cyclobutyl ketone
	Cyclobutylethanone
	1-cyclobutylethan-1-one
Inchi:	InChI=1S/C6H10O/c1-5(7)6-3-2-4-6/h6H,2-4H2,1H3
InchiKey:	JPJOOTWNILDNAW-UHFFFAOYSA-N
Formula:	C6H10O
SMILES:	CC(=O)C1CCC1
Mol. weight [g/mol]:	98.14
CAS:	3019-25-8

Physical Properties

Property code	Value	Unit	Source
gf	-80.63	kJ/mol	Joback Method
hf	-213.11	kJ/mol	Joback Method
hfus	8.93	kJ/mol	Joback Method
hvap	35.78	kJ/mol	Joback Method
log10ws	-1.27		Crippen Method
logp	1.375		Crippen Method
mcvol	86.110	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
tb	411.00 ± 1.00	K	NIST Webbook
tb	411.20	K	NIST Webbook
tb	410.00	K	NIST Webbook
tc	602.85	K	Joback Method
tf	221.73	K	Joback Method
vc	0.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	159.35	J/mol×K	401.56	Joback Method
cpg	214.51	J/mol×K	569.30	Joback Method
cpg	204.72	J/mol×K	535.75	Joback Method
cpg	194.34	J/mol×K	502.20	Joback Method
cpg	183.33	J/mol×K	468.66	Joback Method
cpg	171.68	J/mol×K	435.11	Joback Method
cpg	223.73	J/mol×K	602.85	Joback Method
dvisc	0.0004148	Pa×s	401.56	Joback Method
dvisc	0.0004890	Pa×s	371.59	Joback Method
dvisc	0.0005933	Pa×s	341.62	Joback Method
dvisc	0.0007472	Pa×s	311.64	Joback Method
dvisc	0.0009883	Pa×s	281.67	Joback Method
dvisc	0.0013973	Pa×s	251.70	Joback Method
dvisc	0.0021693	Pa×s	221.73	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=C3019258&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume