Ethanone, 1-cyclopentyl-

Other names:	Ketone, cyclopentyl methyl
	Cyclopentyl methyl ketone
	Cyclopentylethanone
	Acetylcyclopentane
	Methyl cyclopentyl ketone
	1-cyclopentyl ethanone
Inchi:	InChI=1S/C7H12O/c1-6(8)7-4-2-3-5-7/h7H,2-5H2,1H3
InchiKey:	LKENTYLPIUIMFG-UHFFFAOYSA-N
Formula:	C7H12O
SMILES:	CC(=O)C1CCCC1
Mol. weight [g/mol]:	112.17
CAS:	6004-60-0

Physical Properties

Property code	Value	Unit	Source
gf	-84.31	kJ/mol	Joback Method
hf	-239.91	kJ/mol	Joback Method
hfus	9.42	kJ/mol	Joback Method
hvap	38.18	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.766		Crippen Method
mcvol	100.200	ml/mol	McGowan Method
pc	3686.49	kPa	Joback Method
rinpol	933.30		NIST Webbook
rinpol	896.00		NIST Webbook
ripol	1203.00		NIST Webbook
tb	428.71	K	Joback Method
tc	636.28	K	Joback Method
tf	229.48	K	Joback Method
vc	0.374	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	197.08	J/mol×K	428.71	Joback Method
cpg	261.96	J/mol×K	601.69	Joback Method
cpg	250.43	J/mol×K	567.09	Joback Method
cpg	238.20	J/mol×K	532.50	Joback Method
cpg	225.25	J/mol×K	497.90	Joback Method
cpg	211.55	J/mol×K	463.31	Joback Method
cpg	272.82	J/mol×K	636.28	Joback Method
dvisc	0.0003843	Pa×s	428.71	Joback Method
dvisc	0.0004792	Pa×s	395.50	Joback Method
dvisc	0.0006222	Pa×s	362.30	Joback Method
dvisc	0.0008515	Pa×s	329.09	Joback Method
dvisc	0.0012504	Pa×s	295.89	Joback Method
dvisc	0.0020234	Pa×s	262.69	Joback Method
dvisc	0.0037636	Pa×s	229.48	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	431.80 ± 0.80	K	2.70	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6004600&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume