2-Propanone, 1-cyclopentyl-

Other names:	Cyclopentylacetone
	3-Cyclopentylpropanone
	Cyclopentyl-2-propanone
	1-Cyclopentyl-2-propanone
	2-Propanone, cyclopentyl-
Inchi:	InChI=1S/C8H14O/c1-7(9)6-8-4-2-3-5-8/h8H,2-6H2,1H3
InchiKey:	YYJCNNFQNIAISZ-UHFFFAOYSA-N
Formula:	C8H14O
SMILES:	CC(=O)CC1CCCC1
Mol. weight [g/mol]:	126.20
CAS:	1122-98-1

Physical Properties

Property code	Value	Unit	Source
gf	-75.89	kJ/mol	Joback Method
hf	-260.55	kJ/mol	Joback Method
hfus	12.01	kJ/mol	Joback Method
hvap	40.41	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	2.156		Crippen Method
mcvol	114.290	ml/mol	McGowan Method
pc	3291.59	kPa	Joback Method
rinpol	1075.00		NIST Webbook
rinpol	1075.00		NIST Webbook
tb	451.59	K	Joback Method
tc	656.66	K	Joback Method
tf	240.75	K	Joback Method
vc	0.430	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.73	J/mol×K	451.59	Joback Method
cpg	308.58	J/mol×K	622.48	Joback Method

cpg	296.15	J/mol×K	588.30	Joback Method
cpg	282.98	J/mol×K	554.12	Joback Method
cpg	269.04	J/mol×K	519.95	Joback Method
cpg	254.30	J/mol×K	485.77	Joback Method
cpg	320.30	J/mol×K	656.66	Joback Method
dvisc	0.0003821	Pa×s	451.59	Joback Method
dvisc	0.0004800	Pa×s	416.45	Joback Method
dvisc	0.0006289	Pa×s	381.31	Joback Method
dvisc	0.0008704	Pa×s	346.17	Joback Method
dvisc	0.0012965	Pa×s	311.03	Joback Method
dvisc	0.0021374	Pa×s	275.89	Joback Method
dvisc	0.0040775	Pa×s	240.75	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	341.50 ± 0.50	K	2.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1122981&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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