

2-Butanone, 4-cyclopentylidene-

Other names:	4-Cyclopentylidene-2-butanone
Inchi:	InChI=1S/C9H14O/c1-8(10)6-7-9-4-2-3-5-9/h7H,2-6H2,1H3
InchiKey:	ZTMAYXUTUHXWGB-UHFFFAOYSA-N
Formula:	C9H14O
SMILES:	CC(=O)CC=C1CCCC1
Mol. weight [g/mol]:	138.21
CAS:	51004-21-8

Physical Properties

Property code	Value	Unit	Source
gf	-14.30	kJ/mol	Joback Method
hf	-184.82	kJ/mol	Joback Method
hfus	13.85	kJ/mol	Joback Method
hvap	43.73	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.466		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
rinpol	1114.00		NIST Webbook
tb	485.78	K	Joback Method
tc	695.70	K	Joback Method
tf	266.62	K	Joback Method
vc	0.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.15	J/molxK	485.78	Joback Method
cpg	332.61	J/molxK	660.71	Joback Method
cpg	320.90	J/molxK	625.72	Joback Method
cpg	308.43	J/molxK	590.74	Joback Method
cpg	295.18	J/molxK	555.75	Joback Method
cpg	281.10	J/molxK	520.77	Joback Method
cpg	343.61	J/molxK	695.70	Joback Method

dvisc	0.0003112	Paxs	485.78	Joback Method
dvisc	0.0003968	Paxs	449.25	Joback Method
dvisc	0.0005282	Paxs	412.73	Joback Method
dvisc	0.0007432	Paxs	376.20	Joback Method
dvisc	0.0011254	Paxs	339.67	Joback Method
dvisc	0.0018834	Paxs	303.15	Joback Method
dvisc	0.0036296	Paxs	266.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51004218&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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