

Cyclopentanone, 2-(1-methylpropyl)-

Other names:	Cyclopentanone, 2-sec-butyl- 2-sec-Butylcyclopentanone 2-(1-methylpropyl)cyclopentanone
Inchi:	InChI=1S/C9H16O/c1-3-7(2)8-5-4-6-9(8)10/h7-8H,3-6H2,1-2H3
InchiKey:	WVPBKXPDHMXIKD-UHFFFAOYSA-N
Formula:	C9H16O
SMILES:	CCC(C)C1CCCC1=O
Mol. weight [g/mol]:	140.22
CAS:	6376-92-7

Physical Properties

Property code	Value	Unit	Source
gf	-63.58	kJ/mol	Joback Method
hf	-311.59	kJ/mol	Joback Method
hfus	8.99	kJ/mol	Joback Method
hvap	39.74	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.402		Crippen Method
mcvol	128.380	ml/mol	McGowan Method
pc	2893.62	kPa	Joback Method
ripol	1128.00		NIST Webbook
tb	487.98	K	Joback Method
tc	701.70	K	Joback Method
tf	255.31	K	Joback Method
vc	0.481	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.72	J/mol×K	487.98	Joback Method
cpg	309.12	J/mol×K	523.60	Joback Method
cpg	325.71	J/mol×K	559.22	Joback Method
cpg	341.50	J/mol×K	594.84	Joback Method
cpg	356.50	J/mol×K	630.46	Joback Method

cpg	370.70	J/mol×K	666.08	Joback Method
cpg	384.13	J/mol×K	701.70	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6376927&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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