Cyclohexanone, 2-methyl-5-(1-methylethyl)-

Other names:	2-Methyl-5-(1-methylethyl)cyclohexanone
	5-Isopropyl-2-methylcyclohexanone
	TETRAHIDROCARVONA
	Carvoisomenthone
Inchi:	InChI=1S/C10H18O/c1-7(2)9-5-4-8(3)10(11)6-9/h7-9H,4-6H2,1-3H3
InchiKey:	GCRTVIUGJCJVDD-UHFFFAOYSA-N
Formula:	C10H18O
SMILES:	CC1CCC(C(C)C)CC1=O
Mol. weight [g/mol]:	154.25
CAS:	59471-80-6

Physical Properties

Property code	Value	Unit	Source
gf	-74.97	kJ/mol	Joback Method
hf	-358.73	kJ/mol	Joback Method
hfus	10.55	kJ/mol	Joback Method
hvap	41.83	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.648		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
rinpol	1150.00		NIST Webbook
tb	510.46	K	Joback Method
tc	728.68	K	Joback Method
tf	258.82	K	Joback Method
vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.98	J/mol×K	510.46	Joback Method
cpg	358.78	J/mol×K	546.83	Joback Method
cpg	377.66	J/mol×K	583.20	Joback Method
cpg	395.62	J/mol×K	619.57	Joback Method

cpg	412.65	J/mol×K	655.94	Joback Method
cpg	428.75	J/mol×K	692.31	Joback Method
cpg	443.91	J/mol×K	728.68	Joback Method

Sources

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=C59471806&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume