Cyclohexanone, 3-(1-methylethyl)

Other names: 3-Isopropylcyclohexanone
Inchi: InChI=1S/C9H16O/c1-7(2)8-4-3-5-9(10)6-8/h7-8H,3-6H2,1-2H3
InchiKey: AFFBXUKVORMWSC-UHFFFAOYSA-N
Formula: C9H16O
SMILES: CC(C)C1CCCC(=O)C1
Mol. weight [g/mol]: 140.22

Physical Properties

Property code	Value	Unit	Source
gf	-75.68	kJ/mol	Joback Method
hf	-317.75	kJ/mol	Joback Method
hfus	6.89	kJ/mol	Joback Method
hvap	39.92	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.402		Crippen Method
mcvol	128.380	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
rinpol	1172.00		NIST Webbook
rinpol	1172.00		NIST Webbook
tb	492.25	K	Joback Method
tc	714.29	K	Joback Method
tf	251.79	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.68	J/mol×K	492.25	Joback Method
cpg	310.17	J/mol×K	529.26	Joback Method
cpg	327.79	J/mol×K	566.26	Joback Method
cpg	344.53	J/mol×K	603.27	Joback Method
cpg	360.40	J/mol×K	640.28	Joback Method
cpg	375.38	J/mol×K	677.29	Joback Method
cpg	389.49	J/mol×K	714.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R96123&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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