Cyclohexanone, 2-(1-methylethylidene)-

Other names: Cyclohexanone, 2-isopropylidene-
2-Isopropylidenecyclohexanone
Inchi: InChI=1S/C9H14O/c1-7(2)8-5-3-4-6-9(8)10/h3-6H2,1-2H3
InchiKey: MMTBDIDPDFBJIC-UHFFFAOYSA-N
Formula: C9H14O
SMILES: CC(C)=C1CCCCC1=O
Mol. weight [g/mol]: 138.21
CAS: 13747-73-4

Physical Properties

Property code	Value	Unit	Source
gf	-28.62	kJ/mol	Joback Method
hf	-225.89	kJ/mol	Joback Method
hfus	8.35	kJ/mol	Joback Method
hvap	41.48	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.466		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	3173.97	kPa	Joback Method
rinpol	1099.00		NIST Webbook
rinpol	1099.00		NIST Webbook
tb	503.88	K	Joback Method
tc	733.15	K	Joback Method
tf	267.43	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.19	J/mol×K	503.88	Joback Method
cpg	290.87	J/mol×K	542.09	Joback Method
cpg	306.71	J/mol×K	580.30	Joback Method
cpg	321.70	J/mol×K	618.52	Joback Method
cpg	335.86	J/mol×K	656.73	Joback Method

cpg	349.19	J/mol×K	694.94	Joback Method
cpg	361.70	J/mol×K	733.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13747734&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