5-Methyl-2-(1-methylethenylidene)cyclohexanone

Inchi: InChI=1S/C10H16O/c1-7(2)9-5-4-8(3)6-10(9)11/h8H,4-6H2,1-3H3
InchiKey: NZGWDASTMWDZIW-UHFFFAOYSA-N
Formula: C10H16O
SMILES: CC(C)=C1CCC(C)CC1=O
Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
gf	-27.91	kJ/mol	Joback Method
hf	-266.87	kJ/mol	Joback Method
hfus	12.01	kJ/mol	Joback Method
hvap	43.40	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.712		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
rinpol	1335.00		NIST Webbook
rinpol	1332.00		NIST Webbook
tb	522.09	K	Joback Method
tc	747.18	K	Joback Method
tf	274.46	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.00	J/mol×K	522.09	Joback Method
cpg	339.06	J/mol×K	559.61	Joback Method
cpg	356.24	J/mol×K	597.12	Joback Method
cpg	372.52	J/mol×K	634.64	Joback Method
cpg	387.93	J/mol×K	672.15	Joback Method
cpg	402.44	J/mol×K	709.67	Joback Method
cpg	416.08	J/mol×K	747.18	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R577269&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume