Cyclohexanone, 2,5,5-trimethyl-3-(1-methylethylidene)-

Other names: Cyclohexanone, 3-isopropylidene-2,5,5-trimethyl-
2,5,5-Trimethyl-3-(1-methylethylidene)cyclohexanone
Inchi: InChI=1S/C12H20O/c1-8(2)10-6-12(4,5)7-11(13)9(10)3/h9H,6-7H2,1-5H3
InchiKey: RFBHAUFEDARVON-UHFFFAOYSA-N
Formula: C12H20O
SMILES: CC(C)=C1CC(C)(C)CC(=O)C1C
Mol. weight [g/mol]: 180.29
CAS: 38696-32-1

Physical Properties

Property code	Value	Unit	Source
gf	-24.27	kJ/mol	Joback Method
hf	-313.25	kJ/mol	Joback Method
hfus	11.97	kJ/mol	Joback Method
hvap	46.39	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	3.348		Crippen Method
mcvol	166.350	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
rinpol	1346.00		NIST Webbook
tb	563.42	K	Joback Method
tc	789.51	K	Joback Method
tf	316.66	K	Joback Method
vc	0.628	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.08	J/mol×K	563.42	Joback Method
cpg	437.94	J/mol×K	601.10	Joback Method
cpg	456.74	J/mol×K	638.78	Joback Method
cpg	474.59	J/mol×K	676.46	Joback Method
cpg	491.57	J/mol×K	714.14	Joback Method
cpg	507.79	J/mol×K	751.82	Joback Method

cpg	523.33	J/mol×K	789.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38696321&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

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