1-Cyclohexanone, 2-methyl-2-(3-methyl-2-oxobutyl)

Other names: 1-Cyclohexanone, 2-methyl-2-(3-methyl-2-oxabutyl)
Inchi: InChI=1S/C12H20O2/c1-9(2)10(13)8-12(3)7-5-4-6-11(12)14/h9H,4-8H2,1-3H3
InchiKey: PAEODPXIMRWAHT-UHFFFAOYSA-N
Formula: C12H20O2
SMILES: CC(C)C(=O)CC1(C)CCCCC1=O
Mol. weight [g/mol]: 196.29

Physical Properties

Property code	Value	Unit	Source
gf	-184.83	kJ/mol	Joback Method
hf	-477.01	kJ/mol	Joback Method
hfus	9.96	kJ/mol	Joback Method
hvap	52.19	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.751		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2465.36	kPa	Joback Method
rinpol	1309.00		NIST Webbook
tb	615.00	K	Joback Method
tc	842.24	K	Joback Method
tf	359.43	K	Joback Method
vc	0.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.30	J/mol×K	615.00	Joback Method
cpg	480.35	J/mol×K	652.87	Joback Method
cpg	498.36	J/mol×K	690.75	Joback Method
cpg	515.42	J/mol×K	728.62	Joback Method
cpg	531.66	J/mol×K	766.49	Joback Method
cpg	547.16	J/mol×K	804.37	Joback Method
cpg	562.03	J/mol×K	842.24	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=U196694&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