Cyclohexanone, 3-(3,3-dimethylbutyl)-

Other names: 3-[3,3-Dimethylbutyl]-cyclohexanone
Inchi: InChI=1S/C12H22O/c1-12(2,3)8-7-10-5-4-6-11(13)9-10/h10H,4-9H2,1-3H3
InchiKey: VRNWCRVRHPXEIV-UHFFFAOYSA-N
Formula: C12H22O
SMILES: CC(C)(C)CCC1CCCC(=O)C1
Mol. weight [g/mol]: 182.30
CAS: 40564-94-1

Physical Properties

Property code	Value	Unit	Source
gf	-45.14	kJ/mol	Joback Method
hf	-383.14	kJ/mol	Joback Method
hfus	10.77	kJ/mol	Joback Method
hvap	45.69	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.572		Crippen Method
mcvol	170.650	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
ripol	1727.00		NIST Webbook
tb	558.10	K	Joback Method
tc	777.82	K	Joback Method
tf	303.02	K	Joback Method
vc	0.636	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.89	J/mol×K	558.10	Joback Method
cpg	461.42	J/mol×K	594.72	Joback Method
cpg	481.72	J/mol×K	631.34	Joback Method
cpg	500.82	J/mol×K	667.96	Joback Method
cpg	518.75	J/mol×K	704.58	Joback Method
cpg	535.53	J/mol×K	741.20	Joback Method
cpg	551.20	J/mol×K	777.82	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=C40564941&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume