

Cyclohexanone, 4-(1,1-dimethylpropyl)-

Other names:	Cyclohexanone, 4-tert-pentyl- 4-(2-Methyl-sec-butyl)cyclohexanone p-tert-Amylcyclohexanone 4-tert-Amylcyclohexanone 4-(1,1-Dimethylpropyl)cyclohexanone 4-tert-Pentylcyclohexanone NSC 21167
Inchi:	InChI=1S/C11H20O/c1-4-11(2,3)9-5-7-10(12)8-6-9/h9H,4-8H2,1-3H3
InchiKey:	DCSKAMGZSIRJAQ-UHFFFAOYSA-N
Formula:	C11H20O
SMILES:	CCC(C)(C)C1CCC(=O)CC1
Mol. weight [g/mol]:	168.28
CAS:	16587-71-6

Physical Properties

Property code	Value	Unit	Source
gf	-53.56	kJ/mol	Joback Method
hf	-362.50	kJ/mol	Joback Method
hfus	8.18	kJ/mol	Joback Method
hvap	43.46	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	3.182		Crippen Method
mvol	156.560	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
ripol	1800.00		NIST Webbook
tb	535.22	K	Joback Method
tc	758.91	K	Joback Method
tf	291.75	K	Joback Method
vc	0.581	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.62	J/mol×K	535.22	Joback Method

cpg	410.62	J/mol×K	572.50	Joback Method
cpg	430.43	J/mol×K	609.78	Joback Method
cpg	449.06	J/mol×K	647.06	Joback Method
cpg	466.54	J/mol×K	684.35	Joback Method
cpg	482.91	J/mol×K	721.63	Joback Method
cpg	498.19	J/mol×K	758.91	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C16587716&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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