

Cyclohexanone, 3,3,5,5-tetramethyl-

Other names:	3,3,5,5-Tetramethylcyclohexanone
Inchi:	InChI=1S/C10H18O/c1-9(2)5-8(11)6-10(3,4)7-9/h5-7H2,1-4H3
InchiKey:	OQJMHUOCLRCSED-UHFFFAOYSA-N
Formula:	C10H18O
SMILES:	CC1(C)CC(=O)CC(C)(C)C1
Mol. weight [g/mol]:	154.25
CAS:	14376-79-5

Physical Properties

Property code	Value	Unit	Source
gf	-83.51	kJ/mol	Joback Method
hf	-322.97	kJ/mol	Joback Method
hfus	1.48	kJ/mol	Joback Method
hvap	39.92	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.792		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
tb	511.38	K	Joback Method
tc	743.60	K	Joback Method
tf	321.62	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.78	J/mol×K	511.38	Joback Method
cpg	358.04	J/mol×K	550.08	Joback Method
cpg	376.04	J/mol×K	588.79	Joback Method
cpg	392.97	J/mol×K	627.49	Joback Method
cpg	409.03	J/mol×K	666.19	Joback Method
cpg	424.42	J/mol×K	704.90	Joback Method
cpg	439.34	J/mol×K	743.60	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.33507e+01
Coeff. B	-3.64746e+03
Coeff. C	-7.31030e+01
Temperature range (K), min.	352.32
Temperature range (K), max.	526.81

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14376795&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point
vc: Critical Volume

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