

Cyclohexanone, 4-(1,1-dimethylethyl)-

Other names:	4-t-Butylcyclohexanone 4-tert-Butylcyclohexanone C 64 Cyclohexanone, 4-tert-butyl- Cyclohexanone, p-tert-butyl- NSC 73717 p-tert-Butylcyclohexanone «gamma»-tert-Butylcyclohexanone Â«gammaÂ»-tert-Butylcyclohexanone
Inchi:	InChI=1S/C10H18O/c1-10(2,3)8-4-6-9(11)7-5-8/h8H,4-7H2,1-3H3
InchiKey:	YKFKEYKJGVSEIX-UHFFFAOYSA-N
Formula:	C10H18O
SMILES:	CC(C)(C)C1CCC(=O)CC1
Mol. weight [g/mol]:	154.25
CAS:	98-53-3

Physical Properties

Property code	Value	Unit	Source
gf	-61.98	kJ/mol	Joback Method
hf	-341.86	kJ/mol	Joback Method
hfus	5.59	kJ/mol	Joback Method
hvap	41.23	kJ/mol	Joback Method
ie	9.04	eV	NIST Webbook
log10ws	-2.70		Crippen Method
logp	2.792		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2715.50	kPa	Joback Method
rinpol	1208.00		NIST Webbook
rinpol	1208.00		NIST Webbook
ripol	1645.00		NIST Webbook
tb	512.34	K	Joback Method
tc	740.09	K	Joback Method
tf	321.20 ± 3.00	K	NIST Webbook
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.04	J/mol×K	512.34	Joback Method
cpg	361.38	J/mol×K	550.30	Joback Method
cpg	380.56	J/mol×K	588.26	Joback Method
cpg	398.61	J/mol×K	626.21	Joback Method
cpg	415.55	J/mol×K	664.17	Joback Method
cpg	431.39	J/mol×K	702.13	Joback Method
cpg	446.18	J/mol×K	740.09	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	387.70	K	2.70	NIST Webbook
tbrp	364.20	K	1.00	NIST Webbook
tbrp	384.00 ± 1.00	K	2.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.38300e+01
Coeff. B	-3.83144e+03
Coeff. C	-7.48620e+01
Temperature range (K), min.	357.78
Temperature range (K), max.	524.64

Sources

The Yaws Handbook of Vapor
Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
<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=C98533&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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