Cyclohexanone, 2,2,6-trimethyl-

Other names:	1,1,3-Trimethyl-2-cyclohexanone
	2,2,6-Trimethylcyclohexan-1-one
	2,2,6-Trimethylcyclohexanone
	2,6,6-Trimethylcyclohexanone
Inchi:	InChI=1S/C9H16O/c1-7-5-4-6-9(2,3)8(7)10/h7H,4-6H2,1-3H3
InchiKey:	ZPVOLGVTNLDBFI-UHFFFAOYSA-N
Formula:	C9H16O
SMILES:	CC1CCCC(C)(C)C1=O
Mol. weight [g/mol]:	140.22
CAS:	2408-37-9

Physical Properties

Property code	Value	Unit	Source
gf	-86.44	kJ/mol	Joback Method
hf	-317.57	kJ/mol	Joback Method
hfus	5.18	kJ/mol	Joback Method
hvap	38.84	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.402		Crippen Method
mcvol	128.380	ml/mol	McGowan Method
pc	2986.06	kPa	Joback Method
rinpol	1022.90		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	1026.00		NIST Webbook
rinpol	1012.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	1012.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1029.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1011.00		NIST Webbook
rinpol	1035.90		NIST Webbook
rinpol	1017.00		NIST Webbook
rinpol	1011.00		NIST Webbook
rinpol	1027.00		NIST Webbook

rinpol	1008.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1013.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1016.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1022.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1035.00		NIST Webbook
ripol	1335.00		NIST Webbook
ripol	1320.00		NIST Webbook
ripol	1328.00		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1300.00		NIST Webbook
ripol	1307.00		NIST Webbook
ripol	1333.00		NIST Webbook
ripol	1336.00		NIST Webbook
ripol	1327.00		NIST Webbook
ripol	1328.00		NIST Webbook
ripol	1320.00		NIST Webbook
ripol	1320.00		NIST Webbook
ripol	1317.00		NIST Webbook
ripol	1308.00		NIST Webbook
ripol	1308.00		NIST Webbook
ripol	1310.00		NIST Webbook
ripol	1323.00		NIST Webbook
ripol	1323.00		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1312.00		NIST Webbook
ripol	1284.00		NIST Webbook
ripol	1307.00		NIST Webbook
ripol	1303.00		NIST Webbook
tb	451.70	K	NIST Webbook
tc	714.57	K	Joback Method
tf	286.45	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.44	J/mol×K	488.26	Joback Method
cpg	310.90	J/mol×K	525.98	Joback Method
cpg	328.31	J/mol×K	563.70	Joback Method
cpg	344.77	J/mol×K	601.42	Joback Method
cpg	360.36	J/mol×K	639.14	Joback Method
cpg	375.16	J/mol×K	676.85	Joback Method
cpg	389.26	J/mol×K	714.57	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44436e+01
Coeff. B	-3.78265e+03
Coeff. C	-6.67090e+01
Temperature range (K), min.	333.92
Temperature range (K), max.	480.92

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2408379&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

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume