Cyclohexanone, 3,3,5-trimethyl-

Other names: (dl) 3,5,5-trimethylcyclohexanone
3,3,5-Trimethylcyclohexan-1-one
3,3,5-Trimethylcyclohexanone
3,3,5-trimethyi-cyclohexanone
Dihydroisophorone

Inchi: InChI=1S/C9H16O/c1-7-4-8(10)6-9(2,3)5-7/h7H,4-6H2,1-3H3

InchiKey: POSWICCRDBKBMH-UHFFFAOYSA-N

Formula: C9H16O

SMILES: CC1CC(=O)CC(C)(C)C1

Mol. weight [g/mol]: 140.22

CAS: 873-94-9

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	1285.00		NIST Webbook
rinpol	1285.00		NIST Webbook
tb	488.26	K	Joback Method
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
hvapt	39.30	kJ/mol	443.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38745e+01
Coeff. B	-3.70503e+03
Coeff. C	-6.96280e+01
Temperature range (K), min.	305.72
Temperature range (K), max.	502.31

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C873949&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
hvapt: Enthalpy of vaporization at a given temperature

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume