Tetrahydrocarvone

Other names:	Cyclohexanone, 2-methyl-5-(1-methylethyl)-, trans- p-Menthan-2-one, trans- trans-p-Menthan-2-one trans-5-Isopropyl-2-methylcyclohexanone Carvomenthone trans-Cyclohexanone, 2-methyl-5-(1-methylethyl)- 5-Isopropyl-2-methylcyclohexanone, trans- trans-5-isopropyl-2-methylcyclohexan-1-one
Inchi:	InChI=1S/C10H18O/c1-7(2)9-5-4-8(3)10(11)6-9/h7-9H,4-6H2,1-3H3/t8-,9-/m1/s1
InchiKey:	GCRTVIUGJCJVDD-RKDXNWHRSA-N
Formula:	C10H18O
SMILES:	CC1CCC(C(C)C)CC1=O
Mol. weight [g/mol]:	154.25
CAS:	499-70-7

Physical Properties

Property code	Value	Unit	Source
gf	-74.97	kJ/mol	Joback Method
hf	-358.73	kJ/mol	Joback Method
hfus	10.55	kJ/mol	Joback Method
hvap	41.83	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.648		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
rinpol	1178.00		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1185.90		NIST Webbook
rinpol	1193.00		NIST Webbook
rinpol	1181.00		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1208.00		NIST Webbook
ripol	1552.00		NIST Webbook
ripol	1552.00		NIST Webbook
tb	510.46	K	Joback Method
tc	728.68	K	Joback Method
tf	258.82	K	Joback Method

vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.98	J/mol×K	510.46	Joback Method
cpg	358.78	J/mol×K	546.83	Joback Method
cpg	377.66	J/mol×K	583.20	Joback Method
cpg	395.62	J/mol×K	619.57	Joback Method
cpg	412.65	J/mol×K	655.94	Joback Method
cpg	428.75	J/mol×K	692.31	Joback Method
cpg	443.91	J/mol×K	728.68	Joback Method

Sources

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=C499707&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
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