Ethanone, 1-(1,4-dimethyl-3-cyclohexen-1-yl)-

Other names:	1,4-Dimethyl-«delta»-3-tetrahydroacetophenone
	1,4-Dimethyl-3-cyclohexenyl methyl ketone
	1-(1,4-Dimethyl-3-cyclohexen-1-yl)ethanone
	1,4-Dimethyl-cyclohex-3-enyl methyl ketone
	1,4-Dimethyl-4-acetyl-1-cyclohexene
	1,4-Dimethyl-4-acetylcyclohexene
	1-(1,4-Dimethyl)-3-cyclohexen-1-el)ethanone
	1-(1,4-dimethylcyclohex-3-en-1-yl)ethan-1-one
Inchi:	InChI=1S/C10H16O/c1-8-4-6-10(3,7-5-8)9(2)11/h4H,5-7H2,1-3H3
InchiKey:	BIUSXTISNNLMOR-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	CC(=O)C1(C)CC=C(C)CC1
Mol. weight [g/mol]:	152.23
CAS:	43219-68-7

Physical Properties

Property code	Value	Unit	Source
gf	-56.31	kJ/mol	Joback Method
hf	-246.44	kJ/mol	Joback Method
hfus	9.62	kJ/mol	Joback Method
hvap	44.83	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.712		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
rinpol	1156.00		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1126.00		NIST Webbook
ripol	1530.00		NIST Webbook
ripol	1504.00		NIST Webbook
ripol	1491.00		NIST Webbook
ripol	1491.00		NIST Webbook
ripol	1505.00		NIST Webbook
ripol	1530.00		NIST Webbook

ripol	1504.00		NIST Webbook
tb	506.00	K	Joback Method
tc	725.51	K	Joback Method
tf	296.95	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.05	J/mol×K	506.00	Joback Method
cpg	328.76	J/mol×K	542.59	Joback Method
cpg	344.39	J/mol×K	579.17	Joback Method
cpg	359.03	J/mol×K	615.76	Joback Method
cpg	372.81	J/mol×K	652.34	Joback Method
cpg	385.84	J/mol×K	688.93	Joback Method
cpg	398.24	J/mol×K	725.51	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C43219687&Units=SI
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
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