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

Inchi: InChI=1S/C10H16O/c1-8-5-4-6-10(3,7-8)9(2)11/h5H,4,6-7H2,1-3H3
InchiKey: NGMHFVSDLMVOLY-UHFFFAOYSA-N
Formula: C10H16O
SMILES: CC(=O)C1(C)CCC=C(C)C1
Mol. weight [g/mol]: 152.23
CAS: 51733-68-7

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
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=C51733687&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume