2-Cyclohexen-1-one, 3,5,5-trimethyl-4-methylene

Other names: 3,5,5-Trimethyl-4-methylene-cyclohex-2-enone
Inchi: InChI=1S/C10H14O/c1-7-5-9(11)6-10(3,4)8(7)2/h5H,2,6H2,1,3-4H3
InchiKey: MCGQFKNFKWPWAA-UHFFFAOYSA-N
Formula: C10H14O
SMILES: C=C1C(C)=CC(=O)CC1(C)C
Mol. weight [g/mol]: 150.22
CAS: 20548-00-9

Physical Properties

Property code	Value	Unit	Source
gf	3.10	kJ/mol	Joback Method
hf	-187.32	kJ/mol	Joback Method
hfus	6.38	kJ/mol	Joback Method
hvap	42.49	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.488		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
rinpol	1261.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1200.00		NIST Webbook
rinpol	1224.50		NIST Webbook
rinpol	1242.00		NIST Webbook
tb	519.11	K	Joback Method
tc	747.29	K	Joback Method
tf	328.92	K	Joback Method
vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.70	J/mol×K	519.11	Joback Method
cpg	318.43	J/mol×K	557.14	Joback Method
cpg	333.31	J/mol×K	595.17	Joback Method

cpg	347.42	J/mol×K	633.20	Joback Method
cpg	360.84	J/mol×K	671.23	Joback Method
cpg	373.66	J/mol×K	709.26	Joback Method
cpg	385.95	J/mol×K	747.29	Joback Method

Sources

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=C20548009&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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