4-(3-oxobut-1-enylidene)-3,5,5-trimethylcyclohex-

Inchi: InChI=1S/C13H18O2/c1-9-7-11(15)8-13(3,4)12(9)6-5-10(2)14/h6-7H,5,8H2,1-4H3/b12-6
InchiKey: QATWEJYZQLSRAL-WUXMJOGZSA-N
Formula: C13H18O2
SMILES: CC(=O)CC=C1C(C)=CC(=O)CC1(C)C
Mol. weight [g/mol]: 206.28

Physical Properties

Property code	Value	Unit	Source
gf	-108.18	kJ/mol	Joback Method
hf	-370.03	kJ/mol	Joback Method
hfus	17.23	kJ/mol	Joback Method
hvap	56.54	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.837		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2338.29	kPa	Joback Method
rinpol	1673.00		NIST Webbook
rinpol	1673.00		NIST Webbook
rinpol	1683.00		NIST Webbook
tb	649.10	K	Joback Method
tc	877.00	K	Joback Method
tf	409.34	K	Joback Method
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.30	J/mol×K	649.10	Joback Method
cpg	485.19	J/mol×K	687.08	Joback Method
cpg	501.24	J/mol×K	725.07	Joback Method
cpg	516.58	J/mol×K	763.05	Joback Method
cpg	531.29	J/mol×K	801.04	Joback Method
cpg	545.49	J/mol×K	839.02	Joback Method
cpg	559.27	J/mol×K	877.00	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=R218698&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume