4-Hydroxy-2,6,6-trimethyl-3-oxocyclohex-1-ene-1-

Inchi: InChI=1S/C10H14O3/c1-6-7(5-11)10(2,3)4-8(12)9(6)13/h5,8,12H,4H2,1-3H3
InchiKey: PNYLZZYIHSNTOD-UHFFFAOYSA-N
Formula: C10H14O3
SMILES: CC1=C(C=O)C(C)(C)CC(O)C1=O
Mol. weight [g/mol]: 182.22
CAS: 141891-14-7

Physical Properties

Property code	Value	Unit	Source
gf	-303.66	kJ/mol	Joback Method
hf	-541.18	kJ/mol	Joback Method
hfus	14.60	kJ/mol	Joback Method
hvap	66.09	kJ/mol	Joback Method
log10ws	-1.45		Crippen Method
logp	0.862		Crippen Method
mcvol	145.610	ml/mol	McGowan Method
pc	3250.43	kPa	Joback Method
rinpol	1258.00		NIST Webbook
rinpol	1346.20		NIST Webbook
rinpol	1346.20		NIST Webbook
rinpol	1258.00		NIST Webbook
tb	661.10	K	Joback Method
tc	873.46	K	Joback Method
tf	426.34	K	Joback Method
vc	0.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.61	J/mol×K	661.10	Joback Method
cpg	409.63	J/mol×K	696.49	Joback Method
cpg	422.11	J/mol×K	731.89	Joback Method
cpg	434.11	J/mol×K	767.28	Joback Method
cpg	445.69	J/mol×K	802.67	Joback Method

cpg	456.92	J/mol×K	838.06	Joback Method
cpg	467.85	J/mol×K	873.46	Joback Method

Sources

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=C141891147&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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