2-Cyclohexen-1-one, 4-hydroxy-3,5,6-trimethyl-4-(3-oxo-1-butenyl)-

Other names: 4-hydroxy-3,5,6-trimethyl-4-(3-oxo-1-butenyl)-2-cyclohexene-1-one
Inchi: InChI=1S/C13H18O3/c1-8-7-12(15)10(3)11(4)13(8,16)6-5-9(2)14/h5-7,10-11,16H,1-4H3/
InchiKey: IDUJXWVBKIRUFN-AATRIKPKSA-N
Formula: C13H18O3
SMILES: CC(=O)C=CC1(O)C(C)=CC(=O)C(C)C1C
Mol. weight [g/mol]: 222.28
CAS: 77846-84-5

Physical Properties

Property code	Value	Unit	Source
gf	-225.66	kJ/mol	Joback Method
hf	-521.75	kJ/mol	Joback Method
hfus	23.34	kJ/mol	Joback Method
hvap	71.78	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	1.664		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	2453.17	kPa	Joback Method
ripol	2632.00		NIST Webbook
ripol	2632.00		NIST Webbook
tb	729.46	K	Joback Method
tc	943.37	K	Joback Method
tf	446.24	K	Joback Method
vc	0.691	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.59	J/mol×K	729.46	Joback Method
cpg	548.87	J/mol×K	765.11	Joback Method
cpg	563.51	J/mol×K	800.76	Joback Method
cpg	577.60	J/mol×K	836.41	Joback Method
cpg	591.24	J/mol×K	872.07	Joback Method
cpg	604.49	J/mol×K	907.72	Joback Method

cpg	617.45	J/mol×K	943.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77846845&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume