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

Other names: 4-(3-oxo-1-butenyl)-3,5,5-trimethyl-2-cyclohexen-1-one
3,5,5-trimethyl-4-(3-oxo-1-butenyl)-2-cyclohexen-1-one
3,5,5-Trimethyl-4-(3-oxobut-1-en-1-yl)cyclohex-2-enone

Inchi: InChI=1S/C13H18O2/c1-9-7-11(15)8-13(3,4)12(9)6-5-10(2)14/h5-7,12H,8H2,1-4H3/b6-5

InchiKey: MLYOGKJJENFVJN-AATRIKPKSA-N

Formula: C13H18O2

SMILES: CC(=O)C=CC1C(C)=CC(=O)CC1(C)C

Mol. weight [g/mol]: 206.28

CAS: 20194-68-7

Physical Properties

Property code	Value	Unit	Source
gf	-81.13	kJ/mol	Joback Method
hf	-349.18	kJ/mol	Joback Method
hfus	18.18	kJ/mol	Joback Method
hvap	55.41	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.693		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
rinpol	1661.10		NIST Webbook
rinpol	1661.10		NIST Webbook
ripol	2067.00		NIST Webbook
ripol	2078.00		NIST Webbook
ripol	2067.00		NIST Webbook
ripol	2078.00		NIST Webbook
tb	641.95	K	Joback Method
tc	872.71	K	Joback Method
tf	389.66	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	471.42	J/mol×K	641.95	Joback Method
cpg	489.28	J/mol×K	680.41	Joback Method
cpg	506.22	J/mol×K	718.87	Joback Method
cpg	522.33	J/mol×K	757.33	Joback Method
cpg	537.74	J/mol×K	795.79	Joback Method
cpg	552.56	J/mol×K	834.25	Joback Method
cpg	566.89	J/mol×K	872.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20194687&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume