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

Other names: 4-Oxo-«beta»-ionone
4-keto-«beta»-ionone
(E)-2,4,4-trimethyl-3-(3-oxo-1-butenyl)cyclohex-2-en-1-one

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

InchiKey: LNMVXVDYZPDPLE-AATRIKPKSA-N

Formula: C13H18O2

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

Mol. weight [g/mol]: 206.28

CAS: 29790-29-2

Physical Properties

Property code	Value	Unit	Source
gf	-83.05	kJ/mol	Joback Method
hf	-340.31	kJ/mol	Joback Method
hfus	16.72	kJ/mol	Joback Method
hvap	56.38	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.837		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
rinpol	1635.00		NIST Webbook
rinpol	1635.00		NIST Webbook
rinpol	1659.00		NIST Webbook
rinpol	1659.00		NIST Webbook
ripol	2483.00		NIST Webbook
ripol	2483.00		NIST Webbook
ripol	2421.00		NIST Webbook
tb	651.60	K	Joback Method
tc	883.18	K	Joback Method
tf	406.42	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.71	J/mol×K	651.60	Joback Method
cpg	485.89	J/mol×K	690.20	Joback Method
cpg	502.22	J/mol×K	728.79	Joback Method
cpg	517.81	J/mol×K	767.39	Joback Method
cpg	532.78	J/mol×K	805.99	Joback Method
cpg	547.23	J/mol×K	844.58	Joback Method
cpg	561.29	J/mol×K	883.18	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=C29790292&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume