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

Other names: 3-Oxo-7,8-dihydro-«alpha»-ionone
3,5,5-trimethyl-4-(3-oxobutyl)cyclohex-2-en-1-one
3,5,5-Trimethyl-4-(3-oxobutyl)cyclohex-2-enone
Inchi: InChI=1S/C13H20O2/c1-9-7-11(15)8-13(3,4)12(9)6-5-10(2)14/h7,12H,5-6,8H2,1-4H3
InchiKey: GSTVTHMQXVKNQF-UHFFFAOYSA-N
Formula: C13H20O2
SMILES: CC(=O)CCC1C(C)=CC(=O)CC1(C)C
Mol. weight [g/mol]: 208.30
CAS: 74233-41-3

Physical Properties

Property code	Value	Unit	Source
gf	-161.35	kJ/mol	Joback Method
hf	-466.40	kJ/mol	Joback Method
hfus	17.98	kJ/mol	Joback Method
hvap	55.45	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.917		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2204.15	kPa	Joback Method
rinpol	1682.00		NIST Webbook
rinpol	1681.30		NIST Webbook
rinpol	1682.00		NIST Webbook
rinpol	1699.00		NIST Webbook
rinpol	1681.30		NIST Webbook
tb	637.79	K	Joback Method
tc	859.23	K	Joback Method
tf	394.74	K	Joback Method
vc	0.693	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.64	J/mol×K	637.79	Joback Method

cpg	510.97	J/mol×K	674.70	Joback Method
cpg	528.39	J/mol×K	711.60	Joback Method
cpg	544.99	J/mol×K	748.51	Joback Method
cpg	560.85	J/mol×K	785.42	Joback Method
cpg	576.07	J/mol×K	822.33	Joback Method
cpg	590.72	J/mol×K	859.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74233413&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume