2,4,4-Trimethyl-3-(3-oxobutyl)cyclohex-2-enone

Other names: 3-Oxo-7,8-dihydro-«beta»-ionol
Inchi: InChI=1S/C13H20O2/c1-9(14)5-6-11-10(2)12(15)7-8-13(11,3)4/h5-8H2,1-4H3
InchiKey: QUHPCHDTFDSTTL-UHFFFAOYSA-N
Formula: C13H20O2
SMILES: CC(=O)CCC1=C(C)C(=O)CCC1(C)C
Mol. weight [g/mol]: 208.30
CAS: 72008-46-9

Physical Properties

Property code	Value	Unit	Source
gf	-163.27	kJ/mol	Joback Method
hf	-457.53	kJ/mol	Joback Method
hfus	16.52	kJ/mol	Joback Method
hvap	56.42	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	3.061		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2241.88	kPa	Joback Method
rinpol	1695.00		NIST Webbook
rinpol	1731.00		NIST Webbook
rinpol	1695.00		NIST Webbook
rinpol	1731.00		NIST Webbook
rinpol	1675.00		NIST Webbook
ripol	2661.00		NIST Webbook
ripol	2661.00		NIST Webbook
tb	647.44	K	Joback Method
tc	869.76	K	Joback Method
tf	411.50	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.30	J/mol×K	647.44	Joback Method

cpg	507.96	J/mol×K	684.49	Joback Method
cpg	524.79	J/mol×K	721.55	Joback Method
cpg	540.86	J/mol×K	758.60	Joback Method
cpg	556.27	J/mol×K	795.65	Joback Method
cpg	571.10	J/mol×K	832.70	Joback Method
cpg	585.43	J/mol×K	869.76	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72008469&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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