3-OXO-7,8-DIHYDRO-ALPHA-IONONE

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

Physical Properties

Property code	Value	Unit	Source
hfus	17.98	kJ/mol	Joback Method
logp	2.917		Crippen Method
mcvol	182.010	ml/mol	McGowan 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

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

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74233413&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices