6,7-Dehydro-7,8-dihydro-3-oxo-«alpha»-ionone

Inchi: InChI=1S/C13H18O2/c1-9-7-11(15)8-13(3,4)12(9)6-5-10(2)14/h6-7H,5,8H2,1-4H3/b12-6
InchiKey: QATWEJYZQLSRAL-WUXMJOGZSA-N
Formula: C13H18O2
SMILES: CC(=O)CC=C1C(C)=CC(=O)CC1(C)C
Mol. weight [g/mol]: 206.28

Physical Properties

Property code	Value	Unit	Source
hfus	17.23	kJ/mol	Joback Method
logp	2.837		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
rinpol	1720.00		NIST Webbook
rinpol	1720.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.30	J/mol×K	649.10	Joback Method
cpg	485.19	J/mol×K	687.08	Joback Method
cpg	501.24	J/mol×K	725.07	Joback Method
cpg	516.58	J/mol×K	763.05	Joback Method
cpg	531.29	J/mol×K	801.04	Joback Method
cpg	545.49	J/mol×K	839.02	Joback Method
cpg	559.27	J/mol×K	877.00	Joback Method

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R614987&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
Cheméo Relay (1.0):	

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