Dihydrodehydro-«alpha»-ionone

Inchi: InChI=1S/C13H20O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h5-6H,7-9H2,1-4H3
InchiKey: SQFRYZPEWOZAKJ-UHFFFAOYSA-N
Formula: C13H20O
SMILES: CC(=O)CCC1=C(C)C=CCC1(C)C
Mol. weight [g/mol]: 192.30

Physical Properties

Property code	Value	Unit	Source
hfus	18.23	kJ/mol	Joback Method
logp	3.658		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
rinpol	1419.00		NIST Webbook
rinpol	1419.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.65	J/mol×K	578.78	Joback Method
cpg	453.84	J/mol×K	614.09	Joback Method
cpg	470.09	J/mol×K	649.39	Joback Method
cpg	485.49	J/mol×K	684.70	Joback Method
cpg	500.16	J/mol×K	720.00	Joback Method
cpg	514.19	J/mol×K	755.31	Joback Method
cpg	527.70	J/mol×K	790.61	Joback Method

Sources

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):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R631175&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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