3-Oxo-retro-«alpha»-ionol, isomer # 2

Inchi: InChI=1S/C13H22O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h6,8,11,14H,5,7,9H2,1-4H3
InchiKey: BNZGHWQRSDLGKB-UHFFFAOYSA-N
Formula: C13H22O
SMILES: CC1=CCCC(C)(C)C1=CCC(C)O
Mol. weight [g/mol]: 194.31

Physical Properties

Property code	Value	Unit	Source
hf	-271.56	kJ/mol	Cheméo Relay (1.0)
hfus	16.68	kJ/mol	Joback Method
logp	3.450		Crippen Method
mcvol	180.440	ml/mol	McGowan Method
ripol	2880.00		NIST Webbook
ripol	2880.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.00	J/mol×K	619.15	Joback Method
cpg	493.95	J/mol×K	652.12	Joback Method
cpg	509.12	J/mol×K	685.09	Joback Method
cpg	523.62	J/mol×K	718.06	Joback Method
cpg	537.52	J/mol×K	751.03	Joback Method
cpg	550.94	J/mol×K	784.01	Joback Method
cpg	563.95	J/mol×K	816.98	Joback Method

Sources

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=R588655&Units=SI
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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices