3-oxo-retro-«alpha»-ionol (I)

Inchi: InChI=1S/C13H20O2/c1-9-7-11(15)8-13(3,4)12(9)6-5-10(2)14/h6-7,10,14H,5,8H2,1-4H3
InchiKey: JHWWVZZGBLPJPW-UHFFFAOYSA-N
Formula: C13H20O2
SMILES: CC1=CC(=O)CC(C)(C)C1=CCC(C)O
Mol. weight [g/mol]: 208.30

Physical Properties

Property code	Value	Unit	Source
hfus	16.19	kJ/mol	Joback Method
logp	2.629		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
ripol	2752.00		NIST Webbook
ripol	2752.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.30	J/mol×K	686.97	Joback Method
cpg	524.83	J/mol×K	721.86	Joback Method
cpg	539.71	J/mol×K	756.75	Joback Method
cpg	554.03	J/mol×K	791.64	Joback Method
cpg	567.87	J/mol×K	826.52	Joback Method
cpg	581.31	J/mol×K	861.41	Joback Method
cpg	594.44	J/mol×K	896.30	Joback Method

Sources

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=R335778&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

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices