3-oxoretro-7,8-dehydro-«alpha»-ionol

Inchi: InChI=1S/C14H20O/c1-10-8-11(2)13(7-6-12(3)15)14(4,5)9-10/h6,8,12,15H,1,9H2,2-5H3
InchiKey: HMJCYYDLWBSIQE-UHFFFAOYSA-N
Formula: C14H20O
SMILES: C=C1C=C(C)C(=C=CC(C)O)C(C)(C)C1
Mol. weight [g/mol]: 204.31

Physical Properties

Property code	Value	Unit	Source
gf	193.85	kJ/mol	Joback Method
hf	-50.88	kJ/mol	Joback Method
hfus	20.25	kJ/mol	Joback Method
hvap	64.66	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.381		Crippen Method
mcvol	185.930	ml/mol	McGowan Method
pc	2377.22	kPa	Joback Method
ripol	2630.00		NIST Webbook
ripol	2630.00		NIST Webbook
ripol	2630.00		NIST Webbook
tb	644.46	K	Joback Method
tc	850.76	K	Joback Method
tf	368.47	K	Joback Method
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.48	J/mol×K	644.46	Joback Method
cpg	502.73	J/mol×K	678.84	Joback Method
cpg	517.30	J/mol×K	713.23	Joback Method
cpg	531.27	J/mol×K	747.61	Joback Method
cpg	544.72	J/mol×K	781.99	Joback Method
cpg	557.76	J/mol×K	816.37	Joback Method
cpg	570.46	J/mol×K	850.76	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R326388&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume