cis-3-Oxo-«alpha»-ionol

Inchi: InChI=1S/C13H20O2/c1-9(14)5-6-11-10(2)12(15)7-8-13(11,3)4/h5-6,9,14H,7-8H2,1-4H3/
InchiKey: LWWWERIIOIAWQK-WAYWQWQTSA-N
Formula: C13H20O2
SMILES: CC1=C(C=CC(C)O)C(C)(C)CCC1=O
Mol. weight [g/mol]: 208.30

Physical Properties

Property code	Value	Unit	Source
gf	-93.39	kJ/mol	Joback Method
hf	-385.24	kJ/mol	Joback Method
hfus	15.68	kJ/mol	Joback Method
hvap	65.92	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.629		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
ripol	2657.00		NIST Webbook
ripol	2657.00		NIST Webbook
tb	689.47	K	Joback Method
tc	901.80	K	Joback Method
tf	402.31	K	Joback Method
vc	0.680	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.79	J/mol×K	689.47	Joback Method
cpg	525.56	J/mol×K	724.86	Joback Method
cpg	540.68	J/mol×K	760.25	Joback Method
cpg	555.22	J/mol×K	795.64	Joback Method
cpg	569.29	J/mol×K	831.02	Joback Method
cpg	582.97	J/mol×K	866.41	Joback Method
cpg	596.37	J/mol×K	901.80	Joback Method

Sources

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=R423300&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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