13-hydroxy-3-oxo-«alpha»-ionol

Inchi: InChI=1S/C13H20O3/c1-9-6-11(16)7-13(3,8-14)12(9)5-4-10(2)15/h4-6,10,12,14-15H,7-8
InchiKey: DBWLFDJHMPCEEZ-SNAWJCMRSA-N
Formula: C13H20O3
SMILES: CC1=CC(=O)CC(C)(CO)C1C=CC(C)O
Mol. weight [g/mol]: 224.30

Physical Properties

Property code	Value	Unit	Source
gf	-228.29	kJ/mol	Joback Method
hf	-546.34	kJ/mol	Joback Method
hfus	21.23	kJ/mol	Joback Method
hvap	81.63	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.457		Crippen Method
mcvol	187.880	ml/mol	McGowan Method
pc	2632.55	kPa	Joback Method
rinpol	1860.00		NIST Webbook
rinpol	1941.00		NIST Webbook
tb	772.00	K	Joback Method
tc	973.26	K	Joback Method
tf	446.37	K	Joback Method
vc	0.699	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.14	J/mol×K	772.00	Joback Method
cpg	586.21	J/mol×K	805.54	Joback Method
cpg	599.81	J/mol×K	839.09	Joback Method
cpg	613.03	J/mol×K	872.63	Joback Method
cpg	625.95	J/mol×K	906.17	Joback Method
cpg	638.65	J/mol×K	939.71	Joback Method
cpg	651.20	J/mol×K	973.26	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=R288805&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume