3-hydroxy-5,6-epoxy-«beta»-ionol

Inchi: InChI=1S/C13H22O3/c1-9(14)5-6-13-11(2,3)7-10(15)8-12(13,4)16-13/h5-6,9-10,14-15H,
InchiKey: BVNCCXWAZAZQNM-AATRIKPKSA-N
Formula: C13H22O3
SMILES: CC(O)C=CC12OC1(C)CC(O)CC2(C)C
Mol. weight [g/mol]: 226.31
CAS: 172705-14-5

Physical Properties

Property code	Value	Unit	Source
gf	-145.89	kJ/mol	Joback Method
hf	-491.69	kJ/mol	Joback Method
hfus	19.68	kJ/mol	Joback Method
hvap	77.90	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	1.632		Crippen Method
mcvol	185.620	ml/mol	McGowan Method
pc	2838.39	kPa	Joback Method
rinpol	1685.00		NIST Webbook
rinpol	1723.00		NIST Webbook
rinpol	1723.00		NIST Webbook
ripol	2776.00		NIST Webbook
ripol	2768.00		NIST Webbook
ripol	2776.00		NIST Webbook
ripol	2776.00		NIST Webbook
ripol	2776.00		NIST Webbook
ripol	2767.00		NIST Webbook
tb	721.00	K	Joback Method
tc	919.63	K	Joback Method
tf	459.98	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	571.95	J/mol×K	721.00	Joback Method
cpg	586.37	J/mol×K	754.11	Joback Method
cpg	600.86	J/mol×K	787.21	Joback Method
cpg	615.69	J/mol×K	820.32	Joback Method
cpg	631.11	J/mol×K	853.42	Joback Method
cpg	647.40	J/mol×K	886.53	Joback Method
cpg	664.82	J/mol×K	919.63	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=C172705145&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume