2,3-Dehydro-«alpha»-ionol

Inchi: InChI=1S/C13H20O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h5-9,11-12,14H,1-4H3/b8-7+
InchiKey: BMGXVFDEVRFFSY-BQYQJAHWSA-N
Formula: C13H20O
SMILES: CC1=CC=CC(C)(C)C1C=CC(C)O
Mol. weight [g/mol]: 192.30

Physical Properties

Property code	Value	Unit	Source
gf	61.08	kJ/mol	Joback Method
hf	-198.63	kJ/mol	Joback Method
hfus	18.86	kJ/mol	Joback Method
hvap	61.00	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	3.082		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
rinpol	1662.00		NIST Webbook
rinpol	1662.00		NIST Webbook
tb	611.16	K	Joback Method
tc	812.67	K	Joback Method
tf	318.09	K	Joback Method
vc	0.658	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.12	J/mol×K	611.16	Joback Method
cpg	474.98	J/mol×K	644.75	Joback Method
cpg	490.00	J/mol×K	678.33	Joback Method
cpg	504.29	J/mol×K	711.92	Joback Method
cpg	517.95	J/mol×K	745.50	Joback Method
cpg	531.09	J/mol×K	779.09	Joback Method
cpg	543.82	J/mol×K	812.67	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R615455&Units=SI

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