3-hydroxy-«alpha»-ionol

Inchi: InChI=1S/C13H22O2/c1-9-5-8-12(15)13(3,4)11(9)7-6-10(2)14/h5-7,10-12,14-15H,8H2,1-
InchiKey: STFXUMQLYXABNX-VOTSOKGWSA-N
Formula: C13H22O2
SMILES: CC1=CCC(O)C(C)(C)C1C=CC(C)O
Mol. weight [g/mol]: 210.31

Physical Properties

Property code	Value	Unit	Source
gf	-113.41	kJ/mol	Joback Method
hf	-428.98	kJ/mol	Joback Method
hfus	22.79	kJ/mol	Joback Method
hvap	77.07	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.277		Crippen Method
mcvol	186.310	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
ripol	2656.00		NIST Webbook
ripol	2656.00		NIST Webbook
tb	699.51	K	Joback Method
tc	889.60	K	Joback Method
tf	373.91	K	Joback Method
vc	0.691	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.23	J/mol×K	699.51	Joback Method
cpg	559.81	J/mol×K	731.19	Joback Method
cpg	573.81	J/mol×K	762.87	Joback Method
cpg	587.32	J/mol×K	794.55	Joback Method
cpg	600.42	J/mol×K	826.24	Joback Method
cpg	613.19	J/mol×K	857.92	Joback Method
cpg	625.72	J/mol×K	889.60	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=R220869&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume