3-hydroxy-«beta»-ionol

Inchi: InChI=1S/C13H22O2/c1-9(14)5-6-11-10(2)12(15)7-8-13(11,3)4/h5-6,9,12,14-15H,7-8H2,
InchiKey: OFNWHGQGQMQIGF-AATRIKPKSA-N
Formula: C13H22O2
SMILES: CC1=C(C=CC(C)O)C(C)(C)CCC1O
Mol. weight [g/mol]: 210.31

Physical Properties

Property code	Value	Unit	Source
gf	-115.33	kJ/mol	Joback Method
hf	-420.11	kJ/mol	Joback Method
hfus	21.33	kJ/mol	Joback Method
hvap	78.05	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	2.421		Crippen Method
mcvol	186.310	ml/mol	McGowan Method
pc	2502.50	kPa	Joback Method
ripol	2559.00		NIST Webbook
ripol	2559.00		NIST Webbook
tb	709.16	K	Joback Method
tc	900.33	K	Joback Method
tf	390.67	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.73	J/mol×K	709.16	Joback Method
cpg	555.85	J/mol×K	741.02	Joback Method
cpg	569.46	J/mol×K	772.88	Joback Method
cpg	582.63	J/mol×K	804.74	Joback Method
cpg	595.46	J/mol×K	836.61	Joback Method
cpg	608.02	J/mol×K	868.47	Joback Method
cpg	620.41	J/mol×K	900.33	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=R272914&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