3-Hydroxy-7,8-dihydro-«beta»-ionol

Inchi: InChI=1S/C13H20O2/c1-9-7-11(15)8-13(3,4)12(9)6-5-10(2)14/h7,10-12,14-15H,8H2,1-4H
InchiKey: GGHORLDEHPNAFJ-UHFFFAOYSA-N
Formula: C13H20O2
SMILES: CC1=CC(O)CC(C)(C)C1C#CC(C)O
Mol. weight [g/mol]: 208.30
CAS: 172705-13-4

Physical Properties

Property code	Value	Unit	Source
gf	9.17	kJ/mol	Joback Method
hf	-273.90	kJ/mol	Joback Method
hfus	25.71	kJ/mol	Joback Method
hvap	79.27	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	1.724		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
rinpol	1700.00		NIST Webbook
rinpol	1700.00		NIST Webbook
ripol	2661.00		NIST Webbook
ripol	2726.00		NIST Webbook
ripol	2698.00		NIST Webbook
ripol	2681.00		NIST Webbook
ripol	2681.00		NIST Webbook
ripol	2681.00		NIST Webbook
ripol	2681.00		NIST Webbook
ripol	2676.00		NIST Webbook
ripol	2659.00		NIST Webbook
ripol	2661.00		NIST Webbook
ripol	2653.00		NIST Webbook
ripol	2640.00		NIST Webbook
ripol	2726.00		NIST Webbook
ripol	2698.00		NIST Webbook
ripol	2698.00		NIST Webbook
ripol	2700.00		NIST Webbook
tb	704.35	K	Joback Method
tc	905.06	K	Joback Method

tf	485.09	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.02	J/mol×K	704.35	Joback Method
cpg	537.53	J/mol×K	737.80	Joback Method
cpg	551.48	J/mol×K	771.25	Joback Method
cpg	564.93	J/mol×K	804.71	Joback Method
cpg	577.99	J/mol×K	838.16	Joback Method
cpg	590.73	J/mol×K	871.61	Joback Method
cpg	603.23	J/mol×K	905.06	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=C172705134&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