3-hydroxy-7,8-dehydro-«beta»-ionol

Other names: 3-hydroxy-7,8-didehydro-«beta»-ionone
Inchi: InChI=1S/C13H18O2/c1-9-7-11(15)8-13(3,4)12(9)6-5-10(2)14/h11,15H,7-8H2,1-4H3
InchiKey: SZKRSYBOEULCED-UHFFFAOYSA-N
Formula: C13H18O2
SMILES: CC(=O)C#CC1=C(C)CC(O)CC1(C)C
Mol. weight [g/mol]: 206.28

Physical Properties

Property code	Value	Unit	Source
gf	17.59	kJ/mol	Joback Method
hf	-220.10	kJ/mol	Joback Method
hfus	25.29	kJ/mol	Joback Method
hvap	70.69	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	2.076		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2690.21	kPa	Joback Method
rinpol	1689.00		NIST Webbook
rinpol	1609.00		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1689.00		NIST Webbook
ripol	2770.00		NIST Webbook
ripol	2775.00		NIST Webbook
ripol	2746.00		NIST Webbook
ripol	2715.00		NIST Webbook
ripol	2775.00		NIST Webbook
ripol	2770.00		NIST Webbook
ripol	2770.00		NIST Webbook
ripol	2749.00		NIST Webbook
ripol	2775.00		NIST Webbook
tb	676.13	K	Joback Method
tc	893.43	K	Joback Method
tf	505.96	K	Joback Method
vc	0.666	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.74	J/mol×K	676.13	Joback Method
cpg	493.79	J/mol×K	712.35	Joback Method
cpg	508.17	J/mol×K	748.56	Joback Method
cpg	522.01	J/mol×K	784.78	Joback Method
cpg	535.38	J/mol×K	821.00	Joback Method
cpg	548.40	J/mol×K	857.21	Joback Method
cpg	561.17	J/mol×K	893.43	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=R288850&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume