9-Hydroxymegastigma-4,6-dien-3-one (isomer # 1)

Other names: 6,7-Dehydro-7,8-dihydro-3-oxo-«alpha»-ionol (isomer 1)
Inchi: InChI=1S/C13H20O2/c1-9-7-11(15)8-13(3,4)12(9)6-5-10(2)14/h6-7,10,14H,5,8H2,1-4H3
InchiKey: JHWWVZZGBLPJPW-UHFFFAOYSA-N
Formula: C13H20O2
SMILES: CC1=CC(=O)CC(C)(C)C1=CCC(C)O
Mol. weight [g/mol]: 208.30

Physical Properties

Property code	Value	Unit	Source
gf	-118.52	kJ/mol	Joback Method
hf	-414.96	kJ/mol	Joback Method
hfus	16.19	kJ/mol	Joback Method
hvap	66.09	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.629		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
rinpol	1684.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1721.00		NIST Webbook
ripol	2685.00		NIST Webbook
ripol	2720.00		NIST Webbook
ripol	2715.00		NIST Webbook
ripol	2660.00		NIST Webbook
tb	686.97	K	Joback Method
tc	896.30	K	Joback Method
tf	405.23	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.30	J/mol×K	686.97	Joback Method
cpg	524.83	J/mol×K	721.86	Joback Method

cpg	539.71	J/mol×K	756.75	Joback Method
cpg	554.03	J/mol×K	791.64	Joback Method
cpg	567.87	J/mol×K	826.52	Joback Method
cpg	581.31	J/mol×K	861.41	Joback Method
cpg	594.44	J/mol×K	896.30	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=R184699&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

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