Megastigma-4,6-dien-3-one, 9-hydroxy

Other names: 3-oxo-«alpha»-retroionol II
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-WUXMJOGZSA-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
ripol	2894.00		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=R66960&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