Megastigma-4,6,7-trien-3-one, 9-hydroxy

Inchi: InChI=1S/C13H18O2/c1-9-7-11(15)8-13(3,4)12(9)6-5-10(2)14/h5,7,10,14H,8H2,1-4H3
InchiKey: ZYHHDRRWYJNBAN-UHFFFAOYSA-N
Formula: C13H18O2
SMILES: CC1=CC(=O)CC(C)(C)C1=C=CC(C)O
Mol. weight [g/mol]: 206.28

Physical Properties

Property code	Value	Unit	Source
gf	9.76	kJ/mol	Joback Method
hf	-252.18	kJ/mol	Joback Method
hfus	18.32	kJ/mol	Joback Method
hvap	66.52	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.394		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2659.77	kPa	Joback Method
rinpol	1594.00		NIST Webbook
tb	690.24	K	Joback Method
tc	909.56	K	Joback Method
tf	411.74	K	Joback Method
vc	0.663	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.69	J/mol×K	690.24	Joback Method
cpg	504.00	J/mol×K	726.79	Joback Method
cpg	518.66	J/mol×K	763.35	Joback Method
cpg	532.76	J/mol×K	799.90	Joback Method
cpg	546.37	J/mol×K	836.46	Joback Method
cpg	559.57	J/mol×K	873.01	Joback Method
cpg	572.44	J/mol×K	909.56	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=R66956&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume