(6E,8E)-4,6,8-megastigmatrien-3-one

Inchi: InChI=1S/C13H18O/c1-5-6-7-12-10(2)8-11(14)9-13(12,3)4/h5-8H,9H2,1-4H3/b6-5+,12-7
InchiKey: CBQXHTWJSZXYSK-DVIJZSFDSA-N
Formula: C13H18O
SMILES: CC=CC=C1C(C)=CC(=O)CC1(C)C
Mol. weight [g/mol]: 190.28

Physical Properties

Property code	Value	Unit	Source
gf	100.96	kJ/mol	Joback Method
hf	-140.23	kJ/mol	Joback Method
hfus	15.83	kJ/mol	Joback Method
hvap	49.76	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.434		Crippen Method
mcvol	171.840	ml/mol	McGowan Method
pc	2313.61	kPa	Joback Method
rinpol	1582.00		NIST Webbook
tb	599.39	K	Joback Method
tc	830.25	K	Joback Method
tf	354.33	K	Joback Method
vc	0.650	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.35	J/mol×K	599.39	Joback Method
cpg	445.16	J/mol×K	637.87	Joback Method
cpg	462.00	J/mol×K	676.34	Joback Method
cpg	478.00	J/mol×K	714.82	Joback Method
cpg	493.28	J/mol×K	753.29	Joback Method
cpg	507.98	J/mol×K	791.77	Joback Method
cpg	522.21	J/mol×K	830.25	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=R288865&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