Megastigma-6(Z),8(E)-dien-4-one

Inchi: InChI=1S/C13H20O/c1-5-6-7-11-10(2)12(14)8-9-13(11,3)4/h5-7,10H,8-9H2,1-4H3/b6-5+
InchiKey: YYXHVEGUQLRLSY-VLHCFCLRSA-N
Formula: C13H20O
SMILES: CC=CC=C1C(C)C(=O)CCC1(C)C
Mol. weight [g/mol]: 192.30

Physical Properties

Property code	Value	Unit	Source
gf	72.92	kJ/mol	Joback Method
hf	-206.88	kJ/mol	Joback Method
hfus	16.07	kJ/mol	Joback Method
hvap	48.49	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.514		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
pc	2197.95	kPa	Joback Method
rinpol	1490.00		NIST Webbook
tb	590.58	K	Joback Method
tc	818.25	K	Joback Method
tf	336.81	K	Joback Method
vc	0.663	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.51	J/mol×K	590.58	Joback Method
cpg	469.24	J/mol×K	628.53	Joback Method
cpg	487.90	J/mol×K	666.47	Joback Method
cpg	505.59	J/mol×K	704.42	Joback Method
cpg	522.44	J/mol×K	742.36	Joback Method
cpg	538.57	J/mol×K	780.31	Joback Method
cpg	554.08	J/mol×K	818.25	Joback Method

Sources

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=R493691&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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