Megastigma-3,5-dien-9-ol

Inchi: InChI=1S/C13H22O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h5-6,11,14H,7-9H2,1-4H3
InchiKey: WPGXAVCJKGSOBD-UHFFFAOYSA-N
Formula: C13H22O
SMILES: CC1=C(CCC(C)O)C(C)(C)CC=C1
Mol. weight [g/mol]: 194.31

Physical Properties

Property code	Value	Unit	Source
gf	-21.06	kJ/mol	Joback Method
hf	-306.98	kJ/mol	Joback Method
hfus	17.19	kJ/mol	Joback Method
hvap	62.01	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.450		Crippen Method
mcvol	180.440	ml/mol	McGowan Method
pc	2324.78	kPa	Joback Method
ripol	2017.00		NIST Webbook
ripol	2017.00		NIST Webbook
tb	616.65	K	Joback Method
tc	811.51	K	Joback Method
tf	339.93	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	477.59	J/mol×K	616.65	Joback Method
cpg	493.27	J/mol×K	649.13	Joback Method
cpg	508.21	J/mol×K	681.60	Joback Method
cpg	522.49	J/mol×K	714.08	Joback Method
cpg	536.19	J/mol×K	746.56	Joback Method
cpg	549.40	J/mol×K	779.04	Joback Method
cpg	562.20	J/mol×K	811.51	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=R637217&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