6,7-megastigmadiene-3,5,9-triol

Inchi: InChI=1S/C12H20O3/c1-11(2)7-9(14)8-12(3,15)10(11)5-4-6-13/h4,9,13-15H,6-8H2,1-3H
InchiKey: OCBHAQAXMWENRQ-UHFFFAOYSA-N
Formula: C12H20O3
SMILES: CC1(C)CC(O)CC(C)(O)C1=C=CCO
Mol. weight [g/mol]: 212.29

Physical Properties

Property code	Value	Unit	Source
gf	-188.51	kJ/mol	Joback Method
hf	-464.77	kJ/mol	Joback Method
hfus	22.93	kJ/mol	Joback Method
hvap	91.07	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	0.992		Crippen Method
mcvol	178.090	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
rinpol	1652.00		NIST Webbook
tb	771.10	K	Joback Method
tc	963.55	K	Joback Method
tf	471.03	K	Joback Method
vc	0.654	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.54	J/mol×K	771.10	Joback Method
cpg	559.61	J/mol×K	803.18	Joback Method
cpg	572.67	J/mol×K	835.25	Joback Method
cpg	585.85	J/mol×K	867.33	Joback Method
cpg	599.28	J/mol×K	899.40	Joback Method
cpg	613.08	J/mol×K	931.48	Joback Method
cpg	627.38	J/mol×K	963.55	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=R434949&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