3,6-dihydroxy-megastigm-7-en-9-ol

Inchi: InChI=1S/C13H24O3/c1-9-7-11(15)8-12(3,4)13(9,16)6-5-10(2)14/h5-6,9-11,14-16H,7-8H
InchiKey: OJGKTHCXUFNMIQ-AATRIKPKSA-N
Formula: C13H24O3
SMILES: CC(O)C=CC1(O)C(C)CC(O)CC1(C)C
Mol. weight [g/mol]: 228.33

Physical Properties

Property code	Value	Unit	Source
gf	-283.76	kJ/mol	Joback Method
hf	-632.62	kJ/mol	Joback Method
hfus	20.82	kJ/mol	Joback Method
hvap	91.34	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	1.472		Crippen Method
mcvol	196.480	ml/mol	McGowan Method
pc	2673.54	kPa	Joback Method
ripol	3100.00		NIST Webbook
ripol	3100.00		NIST Webbook
tb	783.12	K	Joback Method
tc	972.86	K	Joback Method
tf	441.11	K	Joback Method
vc	0.721	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	630.58	J/mol×K	783.12	Joback Method
cpg	645.42	J/mol×K	814.74	Joback Method
cpg	660.20	J/mol×K	846.37	Joback Method
cpg	675.06	J/mol×K	877.99	Joback Method
cpg	690.13	J/mol×K	909.61	Joback Method
cpg	705.57	J/mol×K	941.23	Joback Method
cpg	721.51	J/mol×K	972.86	Joback Method

Sources

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=R332917&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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