Megastigm-7-en-3,9-diol

Other names: megastigm-7-ene-3,9-diol
Inchi: InChI=1S/C13H24O2/c1-9-7-11(15)8-13(3,4)12(9)6-5-10(2)14/h5-6,9-12,14-15H,7-8H2,1
InchiKey: WIYDYJDQKNCJRC-AATRIKPKSA-N
Formula: C13H24O2
SMILES: CC(O)C=CC1C(C)CC(O)CC1(C)C
Mol. weight [g/mol]: 212.33

Physical Properties

Property code	Value	Unit	Source
gf	-141.45	kJ/mol	Joback Method
hf	-495.63	kJ/mol	Joback Method
hfus	23.03	kJ/mol	Joback Method
hvap	75.81	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.357		Crippen Method
mcvol	190.610	ml/mol	McGowan Method
pc	2331.52	kPa	Joback Method
ripol	2585.00		NIST Webbook
ripol	2589.00		NIST Webbook
ripol	2589.00		NIST Webbook
ripol	2585.00		NIST Webbook
tb	690.70	K	Joback Method
tc	878.51	K	Joback Method
tf	356.39	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.30	J/mol×K	690.70	Joback Method
cpg	588.24	J/mol×K	722.00	Joback Method
cpg	603.51	J/mol×K	753.30	Joback Method
cpg	618.20	J/mol×K	784.61	Joback Method
cpg	632.37	J/mol×K	815.91	Joback Method

cpg	646.12	J/mol×K	847.21	Joback Method
cpg	659.52	J/mol×K	878.51	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=R302708&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

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