3-hydroxy-7,8-didehydro-«beta»-ionol

Other names: megastigma-5-en-7-yne-3,9-diol
Inchi: InChI=1S/C13H20O2/c1-9-7-11(15)8-13(3,4)12(9)6-5-10(2)14/h10-11,14-15H,7-8H2,1-4
InchiKey: PJYBCOAMCYWPHQ-UHFFFAOYSA-N
Formula: C13H20O2
SMILES: CC1=C(C#CC(C)O)C(C)(C)CC(O)C1
Mol. weight [g/mol]: 208.30

Physical Properties

Property code	Value	Unit	Source
gf	7.25	kJ/mol	Joback Method
hf	-265.03	kJ/mol	Joback Method
hfus	24.25	kJ/mol	Joback Method
hvap	80.24	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	1.868		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2796.51	kPa	Joback Method
rinpol	1527.00		NIST Webbook
rinpol	1527.00		NIST Webbook
ripol	2763.00		NIST Webbook
ripol	2763.00		NIST Webbook
ripol	2758.00		NIST Webbook
tb	714.00	K	Joback Method
tc	915.68	K	Joback Method
tf	501.85	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.20	J/mol×K	714.00	Joback Method
cpg	533.25	J/mol×K	747.61	Joback Method
cpg	546.79	J/mol×K	781.23	Joback Method
cpg	559.91	J/mol×K	814.84	Joback Method

cpg	572.69	J/mol×K	848.45	Joback Method
cpg	585.23	J/mol×K	882.07	Joback Method
cpg	597.59	J/mol×K	915.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R220918&Units=SI
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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