

3,17Beta-dihydroxy-1,3,5(10)estratrien-16beta-ylactone

InChI: InChI=1S/C20H24O3/c1-20-7-6-15-14-5-3-13(21)8-11(14)2-4-16(15)17(20)9-12-10-18(22)19
InChIKey: FKUBBKBYUHOFTK-UHFFFAOYSA-N

Formula: C20H24O3

SMILES: CC12CCC3c4ccc(O)cc4CCC3C1CC1CC(=O)OC12

Mol. weight [g/mol]: 312.40

CAS: 95696-45-0

Physical Properties

Property code	Value	Unit	Source
gf	54.86	kJ/mol	Joback Method
hf	-424.64	kJ/mol	Joback Method
hfus	38.66	kJ/mol	Joback Method
hvap	83.05	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.790		Crippen Method
mvol	238.770	ml/mol	McGowan Method
pc	2271.90	kPa	Joback Method
tb	890.45	K	Joback Method
tc	1154.59	K	Joback Method
tf	640.75	K	Joback Method
vc	0.850	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	854.85	J/mol×K	890.45	Joback Method
cpg	878.33	J/mol×K	934.47	Joback Method
cpg	902.03	J/mol×K	978.50	Joback Method
cpg	926.37	J/mol×K	1022.52	Joback Method
cpg	951.76	J/mol×K	1066.55	Joback Method
cpg	978.62	J/mol×K	1110.57	Joback Method
cpg	1007.38	J/mol×K	1154.59	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=C95696450&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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