

Epiestriol

Other names:	Estra-1,3,5(10)-triene-3,16,17-triol, (16«beta»,17«beta»)-Actriol Estra-1,3,5(10)-triene-3,16«beta»,17«beta»-triol Estriol (3,16«beta»,17«beta») 16«beta»-Hydroxyestradiol 16«beta»,17«beta»-Estriol 16-epi-Estriol 16-Epiestratriol 3,16«beta»,17«beta»-Estriol Epioestriol Estra-1,3,5(10)-triene-3,16beta,17beta-triol
Inchi:	InChI=1S/C18H24O3/c1-18-7-6-13-12-5-3-11(19)8-10(12)2-4-14(13)15(18)9-16(20)17(18)
InchiKey:	PROQIPRRNZUXQM-KHHDSSOXSA-N
Formula:	C18H24O3
SMILES:	CC12CCC3c4ccc(O)cc4CCC3C1CC(O)C2O
Mol. weight [g/mol]:	288.38
CAS:	547-81-9

Physical Properties

Property code	Value	Unit	Source
gf	-95.37	kJ/mol	Joback Method
hf	-511.26	kJ/mol	Joback Method
hfus	37.11	kJ/mol	Joback Method
hvap	102.98	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	2.580		Crippen Method
mcvol	225.750	ml/mol	McGowan Method
pc	2738.28	kPa	Joback Method
tb	922.87	K	Joback Method
tc	1147.96	K	Joback Method
tf	622.88	K	Joback Method
vc	0.789	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.84	J/mol×K	922.87	Joback Method
cpg	835.77	J/mol×K	960.38	Joback Method
cpg	855.14	J/mol×K	997.90	Joback Method
cpg	875.20	J/mol×K	1035.41	Joback Method
cpg	896.22	J/mol×K	1072.93	Joback Method
cpg	918.44	J/mol×K	1110.44	Joback Method
cpg	942.13	J/mol×K	1147.96	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=C547819&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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