

«alpha»-Estradiol

Other names:	Estra-1,3,5(10)-triene-3,17-diol, (17«alpha»)-17«alpha»-Estradiol Epiestradiol Estra-1,3,5(10)-triene-3,17«alpha»-diol Oestra-1,3,5(10)-triene-3,17«alpha»-diol 1,3,5-Estratriene-3,17«alpha»-diol 17«alpha»-Oestradiol 3,17«alpha»-Dihydroxyestra-1,3,5(10)-triene 3,17«alpha»-Dihydroxyoestra-1,3,5(10)-triene 3,17-Dihydroxyestratriene Estradiol, 17«alpha»- Oestradiol-17«alpha» Estra-1,3,5(10)-triene-3,17alpha-diol 17-Epiestradiol NSC 20293 Epiestrol Estra-1,3,5(10)-triene-3,17-diol
Inchi:	InChI=1S/C18H24O2/c1-18-9-8-14-13-5-3-12(19)10-11(13)2-4-15(14)16(18)6-7-17(18)20
InchiKey:	VOXZDWNPVJITMN-LESVLKBLSA-N
Formula:	C18H24O2
SMILES:	CC12CCC3c4ccc(O)cc4CCC3C1CCC2O
Mol. weight [g/mol]:	272.38
CAS:	57-91-0

Physical Properties

Property code	Value	Unit	Source
gf	49.16	kJ/mol	Joback Method
hf	-338.69	kJ/mol	Joback Method
hfus	31.95	kJ/mol	Joback Method
hvap	86.61	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.609		Crippen Method
mcvol	219.880	ml/mol	McGowan Method
pc	2576.72	kPa	Joback Method
rinpol	2725.10		NIST Webbook
rinpol	2707.40		NIST Webbook
rinpol	2743.90		NIST Webbook

rinpol	2742.90		NIST Webbook
tb	835.36	K	Joback Method
tc	1069.90	K	Joback Method
tf	566.30	K	Joback Method
vc	0.771	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	748.75	J/mol×K	835.36	Joback Method
cpg	768.05	J/mol×K	874.45	Joback Method
cpg	787.26	J/mol×K	913.54	Joback Method
cpg	806.67	J/mol×K	952.63	Joback Method
cpg	826.60	J/mol×K	991.72	Joback Method
cpg	847.32	J/mol×K	1030.81	Joback Method
cpg	869.14	J/mol×K	1069.90	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=C57910&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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