Estradiol Benzoate

Other names:

Estra-1,3,5(10)-triene-3,17-diol (17«beta»)-, 3-benzoate
Estradiol, 3-benzoate
«beta»-Estradiol benzoate
«beta»-Estradiol 3-benzoate
Benovocylin
Benzhormovarine
Benzo-Gynoestryl
Benzoestrofol
Benzofoline
De Graafina
Diffollisterol
Difolliculine
Dimenformon benzoate
Diogyn B
Eston-B
Estradiol monobenzoate
Femestrone
Graafina
Gynecormone
Gynformone
Hidroestron
Hormogynon
Oestroform [BDH]
Ovahormon benzoate
Ovasterol-B
Ovocyclin Benzoate
Ovocyclin M
Ovocyclin-MB
Primogyn B
Progynon benzoate
Progynon B
Recthormone oestradiol
Solestro
Unistradiol
1,3,5(10)-Estratriene-3,17«beta»-diol 3-benzoate
17«beta»-Estradiol benzoate
17«beta»-Estradiol 3-benzoate
Benzoestrofol difolliculin
Dihydroestrin benzoate
Dihydrofolliculin benzoate

	Dimenformone
	Estra-1,3,5(10)-triene-3,17«beta»-diol, 3-benzoate
	Estradiol-17«beta» benzoate
	Estradiol-17«beta» 3-benzoate
	EBZ
	Follicormon
	Follidrin
	Hydroxyestrin benzoate
	MEE
	Oestradiol benzoate
	Oestradiol monobenzoate
	Oestroform
	Primogyn I
	17«beta»-Estradiol monobenzoate
	Benzoate d'oestradiol
	Benzoic acid estradiol
	ODB
	Oestradiol 3-benzoate
	«beta»-Oestradiol benzoate
	«beta»-Oestradiol 3-benzoate
	17-«beta»-Oestradiol 3-benzoate
	1,3,5(10)-Oestratriene-3,17-«beta»-diol 3-benzoate
	Oestraform
	Primogyn boleosum
	Benzestrofol
	Benzogynestryl
	(17«beta»)-Estra-1,3,5(10)-triene-3,17-diol 3-benzoate
	Benztrone
	NSC-9566
	Pelanin benzoate
	17-Hydroxyestra-1(10),2,4-trien-3-yl benzoate, (17«beta»)-
	3-Benzoyloxy-17«beta»-hydroxyestra-1,3,5(10)-triene
	Estrogin
	Folone
	Mesalin
Inchi:	InChI=1S/C25H28O3/c1-25-14-13-20-19-10-8-18(28-24(27)16-5-3-2-4-6-16)15-17(19)7-9
InchiKey:	UYIFTLBWAOGQBI-PPWDSJTCSA-N
Formula:	C25H28O3
SMILES:	CC12CCC3c4ccc(OC(=O)c5ccccc5)cc4CCC3C1CCC2O
Mol. weight [g/mol]:	376.49
CAS:	50-50-0

Physical Properties

Property code	Value	Unit	Source
gf	131.58	kJ/mol	Joback Method
hf	-325.60	kJ/mol	Joback Method
hfus	40.73	kJ/mol	Joback Method
hvap	101.27	kJ/mol	Joback Method
log10ws	-6.81		Crippen Method
logp	5.123		Crippen Method
mcvol	296.320	ml/mol	McGowan Method
pc	1694.90	kPa	Joback Method
tb	1022.85	K	Joback Method
tc	1268.96	K	Joback Method
tf	471.00 ± 1.00	K	NIST Webbook
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1068.08	J/mol×K	1022.85	Joback Method
cpg	1090.64	J/mol×K	1063.87	Joback Method
cpg	1113.61	J/mol×K	1104.89	Joback Method
cpg	1137.29	J/mol×K	1145.91	Joback Method
cpg	1161.96	J/mol×K	1186.92	Joback Method
cpg	1187.93	J/mol×K	1227.94	Joback Method
cpg	1215.48	J/mol×K	1268.96	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C50500&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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