

Estradiol, diacetate

Other names:	Estra-1,3,5(10)-triene-3,17-diol (17«beta»)-, diacetate «beta»-Estradiol diacetate Estradiol-3,17«beta»-diacetate Estradiol-3,17-diacetate 17«beta»-Estradiol diacetate 3,17«beta»-Diacetoxyestra-1,3,5(10)-triene 17«beta»-(Acetyloxy)estra-1,3,5(10)-trien-3-yl acetate 3,17«beta»-di(Acetyloxy)estra-1,3,5(10)-triene Estra-1,3,5(10)-triene-3,17«beta»-diol diacetate NSC 106559 3,17Beta-diacetoxyestra-1,3,5(10)-triene
Inchi:	InChI=1S/C22H28O4/c1-13(23)25-16-5-7-17-15(12-16)4-6-19-18(17)10-11-22(3)20(19)8
InchiKey:	VQHQLBARMFAKSV-UHFFFAOYSA-N
Formula:	C22H28O4
SMILES:	CC(=O)Oc1ccc2c(c1)CCC1C2CCC2(C)C(OC(C)=O)CCC12
Mol. weight [g/mol]:	356.46
CAS:	3434-88-6

Physical Properties

Property code	Value	Unit	Source
gf	-103.19	kJ/mol	Joback Method
hf	-592.78	kJ/mol	Joback Method
hfus	37.62	kJ/mol	Joback Method
hvap	84.79	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	4.400		Crippen Method
mcvol	279.380	ml/mol	McGowan Method
pc	1577.21	kPa	Joback Method
tb	911.64	K	Joback Method
tc	1147.76	K	Joback Method
tf	595.68	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	961.30	J/mol×K	911.64	Joback Method
cpg	982.46	J/mol×K	950.99	Joback Method
cpg	1003.15	J/mol×K	990.35	Joback Method
cpg	1023.59	J/mol×K	1029.70	Joback Method
cpg	1043.99	J/mol×K	1069.05	Joback Method
cpg	1064.55	J/mol×K	1108.41	Joback Method
cpg	1085.50	J/mol×K	1147.76	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C3434886&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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