3,17Beta-diacetoxyestra-1,3,5(10)-triene

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

Physical Properties

Property code	Value	Unit	Source
hfus	37.62	kJ/mol	Joback Method
ie	7.99	eV	Cheméo Relay (1.0)
log10ws	-5.24		Cheméo Relay (1.0)
logp	4.400		Crippen Method
mcvol	279.380	ml/mol	McGowan Method
tf	394.13	K	Cheméo Relay (1.0)

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3434886&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point