

Estra-1,3,5(10)-triene-3,17-diol (17«beta»)-, bis(trifluoroacetate)

Other names:	Estradiol, bis(trifluoroacetate) «beta»-Estradiol, bis(trifluoroacetate) 17-[(2,2,2-Trifluoroacetyl)oxy]estra-1,3,5(10)-trien-3-yl trifluoroacetate
Inchi:	InChI=1S/C22H22F6O4/c1-20-9-8-14-13-5-3-12(31-18(29)21(23,24)25)10-11(13)2-4-15(
InchiKey:	GBPADILCVOCPX-GXAQHZSOSA-N
Formula:	C22H22F6O4
SMILES:	CC12CCC3c4ccc(OC(=O)C(F)(F)F)cc4CCC3C1CCC2OC(=O)C(F)(F)F
Mol. weight [g/mol]:	464.40
CAS:	1549-15-1

Physical Properties

Property code	Value	Unit	Source
gf	-1266.37	kJ/mol	Joback Method
hf	-1786.94	kJ/mol	Joback Method
hfus	41.27	kJ/mol	Joback Method
hvap	77.30	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	5.484		Crippen Method
mcvol	290.000	ml/mol	McGowan Method
pc	1322.31	kPa	Joback Method
rinpol	2327.00		NIST Webbook
rinpol	2354.50		NIST Webbook
rinpol	2286.00		NIST Webbook
tb	900.80	K	Joback Method
tc	1116.03	K	Joback Method
tf	604.06	K	Joback Method
vc	1.145	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1004.36	J/mol×K	900.80	Joback Method
cpg	1022.36	J/mol×K	936.67	Joback Method
cpg	1040.07	J/mol×K	972.54	Joback Method

cpg	1057.67	J/mol×K	1008.42	Joback Method
cpg	1075.39	J/mol×K	1044.29	Joback Method
cpg	1093.44	J/mol×K	1080.16	Joback Method
cpg	1112.01	J/mol×K	1116.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1549151&Units=SI
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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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