1,3,5(10)-Oestratriene-3,17«beta»-diol, 3-non-deriv-17-HFB

Inchi: InChI=1S/C22H23F7O3/c1-19-9-8-14-13-5-3-12(30)10-11(13)2-4-15(14)16(19)6-7-17(19

InchiKey: CCRBPDNGXJRWRQ-DOEOUOAPSA-N

Formula: C22H23F7O3

SMILES: CC12CCC3c4ccc(O)cc4CCC3C1CCC2OC(=O)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 468.40

Physical Properties

Property code	Value	Unit	Source
gf	-1369.41	kJ/mol	Joback Method
hf	-1912.84	kJ/mol	Joback Method
hfus	40.32	kJ/mol	Joback Method
hvap	78.38	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	5.993		Crippen Method
mcvol	290.200	ml/mol	McGowan Method
pc	1415.44	kPa	Joback Method
rinpol	2856.00		NIST Webbook
tb	896.19	K	Joback Method
tc	1114.08	K	Joback Method
tf	634.11	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.87	J/mol×K	896.19	Joback Method
cpg	1043.91	J/mol×K	932.51	Joback Method
cpg	1063.14	J/mol×K	968.82	Joback Method
cpg	1082.85	J/mol×K	1005.14	Joback Method
cpg	1103.34	J/mol×K	1041.45	Joback Method
cpg	1124.93	J/mol×K	1077.77	Joback Method
cpg	1147.90	J/mol×K	1114.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R537221&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume