1,3,5(10)-Oestratriene-2-methoxy-3,16«alpha»,17«beta»-triol-16,17-bis(2,2,3,3,4,4,4-heptafluorobutanoate), 3-non-deriv-16,17-PFP

Inchi: InChI=1S/C25H24F10O6/c1-21-6-5-11-12(4-3-10-7-15(36)16(39-2)8-13(10)11)14(21)9-1

InchiKey: XKCPQLZEMXYPPS-CBPXGTFBSA-N

Formula: C25H24F10O6

SMILES: COc1cc2c(cc1O)CCC1C2CCC2(C)C1CC(OC(=O)C(F)(F)C(F)(F)F)C2OC(=O)C(F)(F)C(F

Mol. weight [g/mol]: 610.44

Physical Properties

Property code	Value	Unit	Source
gf	-2282.00	kJ/mol	Joback Method
hf	-2980.67	kJ/mol	Joback Method
hfus	54.58	kJ/mol	Joback Method
hvap	93.23	kJ/mol	Joback Method
log10ws	-7.43		Crippen Method
logp	6.086		Crippen Method
mcvol	351.090	ml/mol	McGowan Method
pc	1053.46	kPa	Joback Method
rinpol	2544.00		NIST Webbook
tb	1058.43	K	Joback Method
tc	1296.63	K	Joback Method
tf	774.78	K	Joback Method
vc	1.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1321.07	J/mol×K	1058.43	Joback Method
cpg	1345.22	J/mol×K	1098.13	Joback Method
cpg	1370.68	J/mol×K	1137.83	Joback Method
cpg	1397.82	J/mol×K	1177.53	Joback Method
cpg	1427.04	J/mol×K	1217.23	Joback Method
cpg	1458.69	J/mol×K	1256.93	Joback Method
cpg	1493.17	J/mol×K	1296.63	Joback Method

Sources

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=R537132&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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