Estriol, TFA

Inchi: InChI=1S/C24H21F9O6/c1-21-7-6-13-12-5-3-11(37-18(34)22(25,26)27)8-10(12)2-4-14(1
InchiKey: WWJXNFAAIBBBGC-CZLQREIISA-N
Formula: C24H21F9O6
SMILES: CC12CCC3c4ccc(OC(=O)C(F)(F)F)cc4CCC3C1CC(OC(=O)C(F)(F)F)C2OC(=O)C(F)(F)F
Mol. weight [g/mol]: 576.41

Physical Properties

Property code	Value	Unit	Source
gf	-2072.75	kJ/mol	Joback Method
hf	-2690.44	kJ/mol	Joback Method
hfus	52.14	kJ/mol	Joback Method
hvap	86.85	kJ/mol	Joback Method
log10ws	-7.27		Crippen Method
logp	5.568		Crippen Method
mcvol	330.930	ml/mol	McGowan Method
pc	1078.51	kPa	Joback Method
rinpol	2340.00		NIST Webbook
rinpol	2340.00		NIST Webbook
tb	1012.76	K	Joback Method
tc	1239.90	K	Joback Method
tf	698.71	K	Joback Method
vc	1.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1199.91	J/mol×K	1012.76	Joback Method
cpg	1218.65	J/mol×K	1050.62	Joback Method
cpg	1237.57	J/mol×K	1088.47	Joback Method
cpg	1256.91	J/mol×K	1126.33	Joback Method
cpg	1276.93	J/mol×K	1164.19	Joback Method
cpg	1297.87	J/mol×K	1202.05	Joback Method
cpg	1320.00	J/mol×K	1239.90	Joback Method

Sources

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=R305336&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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