17.beta.-16-oxo-Oestradiol, TFA

Inchi: InChI=1S/C22H20F6O5/c1-20-7-6-13-12-5-3-11(32-18(30)21(23,24)25)8-10(12)2-4-14(1
InchiKey: BRYCMNUGPVBHCU-DGMDJVGWSA-N
Formula: C22H20F6O5
SMILES: C[C@]12CC[C@@H]3c4ccc(OC(=O)C(F)(F)F)cc4CCC3[C@@H]1CC(=O)[C@H]2OC(=O
Mol. weight [g/mol]: 478.38

Physical Properties

Property code	Value	Unit	Source
hfus	40.78	kJ/mol	Joback Method
ie	9.07	eV	Cheméo Relay (1.0)
log10ws	-6.31		Cheméo Relay (1.0)
logp	4.663		Crippen Method
mcvol	291.570	ml/mol	McGowan Method
tf	440.48	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1037.78	J/mol×K	968.62	Joback Method
cpg	1055.68	J/mol×K	1006.38	Joback Method
cpg	1073.41	J/mol×K	1044.15	Joback Method
cpg	1091.18	J/mol×K	1081.91	Joback Method
cpg	1109.20	J/mol×K	1119.68	Joback Method
cpg	1127.68	J/mol×K	1157.44	Joback Method
cpg	1146.82	J/mol×K	1195.20	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?Str2File=R523861

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