.alpha.-Estradiol, bis(pentafluoropropionate)

Inchi: InChI=1S/C24H22F10O4/c1-20-9-8-14-13-5-3-12(37-18(35)21(25,26)23(29,30)31)10-11(
InchiKey: JYKXKZJIOJLRNL-UHFFFAOYSA-N
Formula: C24H22F10O4
SMILES: CC12CCC3c4ccc(OC(=O)C(F)(F)C(F)(F)F)cc4CCC3C1CCC2OC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 564.42

Physical Properties

Property code	Value	Unit	Source
hfus	43.95	kJ/mol	Joback Method
ie	9.02	eV	Cheméo Relay (1.0)
log10ws	-8.57		Cheméo Relay (1.0)
logp	6.755		Crippen Method
mcvol	325.260	ml/mol	McGowan Method
tf	387.33	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1155.74	J/mol×K	937.18	Joback Method
cpg	1173.90	J/mol×K	972.60	Joback Method
cpg	1192.06	J/mol×K	1008.01	Joback Method
cpg	1210.47	J/mol×K	1043.43	Joback Method
cpg	1229.38	J/mol×K	1078.85	Joback Method
cpg	1249.04	J/mol×K	1114.26	Joback Method
cpg	1269.71	J/mol×K	1149.68	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=U352227

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