«alpha»-Estradiol, bis(trifluoroacetate)

Inchi: InChI=1S/C22H22F6O4/c1-20-9-8-14-13-5-3-12(31-18(29)21(23,24)25)10-11(13)2-4-15(
InchiKey: GBPADILCVOCPSX-UHFFFAOYSA-N
Formula: C22H22F6O4
SMILES: CC12CCC3c4ccc(OC(=O)C(F)(F)F)cc4CCC3C1CCC2OC(=O)C(F)(F)F
Mol. weight [g/mol]: 464.40

Physical Properties

Property code	Value	Unit	Source
gf	-1266.37	kJ/mol	Joback Method
hf	-1786.94	kJ/mol	Joback Method
hfus	41.27	kJ/mol	Joback Method
hvap	77.30	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	5.484		Crippen Method
mcvol	290.000	ml/mol	McGowan Method
pc	1322.31	kPa	Joback Method
rinpol	2318.10		NIST Webbook
rinpol	2318.10		NIST Webbook
tb	900.80	K	Joback Method
tc	1116.03	K	Joback Method
tf	604.06	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1004.36	J/mol×K	900.80	Joback Method
cpg	1022.36	J/mol×K	936.67	Joback Method
cpg	1040.07	J/mol×K	972.54	Joback Method
cpg	1057.67	J/mol×K	1008.42	Joback Method
cpg	1075.39	J/mol×K	1044.29	Joback Method
cpg	1093.44	J/mol×K	1080.16	Joback Method
cpg	1112.01	J/mol×K	1116.03	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1549151&Units=SI

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