Estra-1,3,5(10)-trien-17-one, 1-methyl-3,6,7-tris[(trifluoroacetyl)oxy]-, (6«alpha»,7«alpha»)-

Other names: 1-Methyl-6«alpha»,7«alpha»-dihydroxyestrone, TFA
Inchi: InChI=1S/C25H21F9O7/c1-9-7-10(39-19(36)23(26,27)28)8-12-15(9)11-5-6-22(2)13(3-4-1
InchiKey: IXDHLXAZUNPBDV-HTUBNKTISA-N
Formula: C25H21F9O7
SMILES: Cc1cc(OC(=O)C(F)(F)F)cc2c1C1CCC3(C)C(=O)CCC3C1C(OC(=O)C(F)(F)F)C2OC(=O)
Mol. weight [g/mol]: 604.42
CAS: 56588-13-7

Physical Properties

Property code	Value	Unit	Source
gf	-2196.55	kJ/mol	Joback Method
hf	-2860.25	kJ/mol	Joback Method
hfus	53.85	kJ/mol	Joback Method
hvap	93.98	kJ/mol	Joback Method
log10ws	-7.38		Crippen Method
logp	5.576		Crippen Method
mcvol	346.590	ml/mol	McGowan Method
pc	1026.63	kPa	Joback Method
rinpol	2520.00		NIST Webbook
tb	1108.44	K	Joback Method
tc	1359.36	K	Joback Method
tf	790.72	K	Joback Method
vc	1.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1294.07	J/mol×K	1108.44	Joback Method
cpg	1314.36	J/mol×K	1150.26	Joback Method
cpg	1335.05	J/mol×K	1192.08	Joback Method
cpg	1356.41	J/mol×K	1233.90	Joback Method
cpg	1378.75	J/mol×K	1275.72	Joback Method
cpg	1402.34	J/mol×K	1317.54	Joback Method
cpg	1427.46	J/mol×K	1359.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56588137&Units=SI
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

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