Testosterone, 3-HFB, 17.beta.-monochloacetate

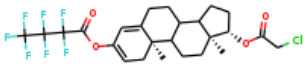
InChI: InChI=1S/C25H28ClF7O4/c1-21-9-7-14(36-20(35)23(27,28)24(29,30)25(31,32)33)11-13(21)3-4-15-16-5-6-18(37-19(34)12-26)22(16,2)10-8-17(15)21/h7,11,15-18H,3-6,8-10,12H2,1-2H3/t15?,16?,17?,18-,21-,22-/m1/s1

InChI Key: WYBQRJXFEKTTGH-FSFORYKRSA-N

Formula: C25H28ClF7O4

SMILES: CC12CCC3C(CCC4=CC(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)=CCC43C)C1CCC2OC(=O)CCl

Molecular Weight: 560.93



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-1478.54	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-2120.87	kJ/mol	Joback Method
$\Delta_{fus} H°$	42.85	kJ/mol	Joback Method
$\Delta_{vap} H°$	83.83	kJ/mol	Joback Method
$logP_{oct/wat}$	6.970		Crippen Method
P_c	1033.90	kPa	Joback Method
T_{boil}	994.34	K	Joback Method
T_c	1220.42	K	Joback Method
T_{fus}	677.18	K	Joback Method
V_c	1.379	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1269.60	J/mol×K	994.34	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C25H28ClF7O4/c1-21-9-7-14(36-20(35)23(27,28)24(29,30)25(31,32)33)11-13(21)3-4-15-16-5-6-18(37-19(34)12-26)22(16,2)10-8-17(15)21/h7,11,15-18H,3-6,8-10,12H2,1-2H3/t15?,16?,17?,18-,21-,22-/m1/s1

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: Enthalpy of vaporization at standard conditions (kJ/mol).
***log*$P_{oct/wat}$**: Octanol/Water partition coefficient .
P_c: Critical Pressure (kPa).
T_{boil}: Normal Boiling Point Temperature (K).
T_c: Critical Temperature (K).
T_{fus}: Normal melting (fusion) point (K).
V_c: Critical Volume (m^3/kg-mol).