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

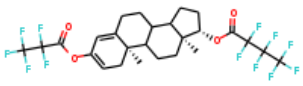
InChI: InChI=1S/C26H26F12O4/c1-20-9-7-13(41-19(40)23(29,30)25(33,34)35)11-12(20)3-4-14-15-5-6-17(21(15,2)10-8-16(14)20)42-18(39)22(27,28)24(31,32)26(36,37)38/h7,11,14-17H,3-6,8-10H2,1-2H3/t14?,15?,16?,17-,20-,21-/m1/s1

InChI Key: USLXJCDJCHXXGL-FVLSIOMWSA-N

Formula: C26H26F12O4

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

Molecular Weight: 630.46



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-2426.56	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-3123.82	kJ/mol	Joback Method
$\Delta_{fus} H°$	41.81	kJ/mol	Joback Method
$\Delta_{vap} H°$	75.00	kJ/mol	Joback Method
$logP_{oct/wat}$	7.93		Crippen Method
P_c	887.88	kPa	Joback Method
T_{boil}	969.68	K	Joback Method
T_c	1187.21	K	Joback Method
T_{fus}	666.32	K	Joback Method
V_c	1.45	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1334.61	J/mol×K	969.68	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C26H26F12O4/c1-20-9-7-13(41-19(40)23(29,30)25(33,34)35)11-12(20)3-4-14-15-5-6-17(21(15,2)10-8-16(14)20)42-18(39)22(27,28)24(31,32)26(36,37)38/h7,11,14-17H,3-6,8-10H2,1-2H3/t14?,15?,16?,17-,20-,21-/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).