Androsta-2,4-diene-3,17-diol, 17-acetate 3-(2,2,3,3,4,4,4-heptafluorobutanoate), (17«beta»)-

Other names: 17-(Acetyloxy)androsta-2,4-dien-3-yl 2,2,3,3,4,4,4-heptafluorobutanoate, (17«beta»)-; Testosterone, 3-HFB, 17«beta»-Ac.

InChI: InChI=1S/C25H29F7O4/c1-13(33)35-19-7-6-17-16-5-4-14-12-15(8-10-21(14,2)18(16)9-11-22(17,19)3)36-20(34)23(26,27)24(28,29)25(30,31)32/h8,12,16-19H,4-7,9-11H2,1-3H3/t16-,17-,18-,19-,21-,22-/m1/s1

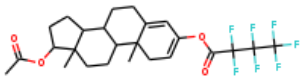
InChI Key: NTZWSZQHFGGWDX-OYSQMQRMSA-N

Formula: C25H29F7O4

SMILES: CC(=O)OC1CCC2C3CCC4=CC(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)=CCC4(C)C3CCC12C

Molecular Weight: 526.48

CAS: 49566-69-0



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-1466.61	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-2105.13	kJ/mol	Joback Method
$\Delta_{fus} H°$	38.65	kJ/mol	Joback Method
$\Delta_{vap} H°$	79.45	kJ/mol	Joback Method
$logP_{oct/wat}$	6.751		Crippen Method
P_c	1058.95	kPa	Joback Method
T_{boil}	956.91	K	Joback Method
T_c	1176.82	K	Joback Method
T_{fus}	647.26	K	Joback Method
V_c	1.331	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1236.02	J/mol×K	956.91	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C25H29F7O4/c1-13(33)35-19-7-6-17-16-5-4-14-12-15(8-10-21(14,2)18(16)9-11-22(17,19)3)36-20(34)23(26,27)24(28,29)25(30,31)32/h8,12,16-19H,4-7,9-11H2,1-3H3/t16-,17-,18-,19-,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).