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)9-1

InchiKey: 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

Mol. weight [g/mol]: 526.48

CAS: 49566-69-0

Physical Properties

Property code	Value	Unit	Source
gf	-1466.61	kJ/mol	Joback Method
hf	-2105.13	kJ/mol	Joback Method
hfus	38.65	kJ/mol	Joback Method
hvap	79.45	kJ/mol	Joback Method
log10ws	-7.99		Crippen Method
logp	6.751		Crippen Method
mcvol	338.340	ml/mol	McGowan Method
pc	1058.95	kPa	Joback Method
rinpol	2566.00		NIST Webbook
tb	956.91	K	Joback Method
tc	1176.82	K	Joback Method
tf	647.26	K	Joback Method
vc	1.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1236.02	J/mol×K	956.91	Joback Method
cpg	1260.76	J/mol×K	993.56	Joback Method
cpg	1286.32	J/mol×K	1030.21	Joback Method
cpg	1313.04	J/mol×K	1066.86	Joback Method
cpg	1341.27	J/mol×K	1103.51	Joback Method
cpg	1371.35	J/mol×K	1140.17	Joback Method

cpg	1403.62	J/mol×K	1176.82	Joback Method

Sources

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=C49566690&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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