

Testosterone, 3-HFB, 17«beta»-PFB

Inchi:	InChI=1S/C30H26F12O4/c1-26-9-7-13(45-25(44)28(36,37)29(38,39)30(40,41)42)11-12(2
InchiKey:	VQRFVWKMQHJHEY-RIUZPASXSA-N
Formula:	C30H26F12O4
SMILES:	CC12CC=C(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)C=C1CCC1C2CCC2(C)C(OC(=O)c3c(F)c(F
Mol. weight [g/mol]:	678.51

Physical Properties

Property code	Value	Unit	Source
gf	-2334.30	kJ/mol	Joback Method
hf	-3009.70	kJ/mol	Joback Method
hfus	59.10	kJ/mol	Joback Method
hvap	92.08	kJ/mol	Joback Method
log10ws	-11.42		Crippen Method
logp	8.740		Crippen Method
mcvol	393.880	ml/mol	McGowan Method
pc	806.16	kPa	Joback Method
rinpol	3020.00		NIST Webbook
rinpol	3020.00		NIST Webbook
tb	1119.24	K	Joback Method
tc	1377.75	K	Joback Method
tf	795.58	K	Joback Method
vc	1.593	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1515.04	J/molxK	1119.24	Joback Method
cpg	1551.62	J/molxK	1162.32	Joback Method
cpg	1591.18	J/molxK	1205.41	Joback Method
cpg	1634.27	J/molxK	1248.49	Joback Method
cpg	1681.44	J/molxK	1291.58	Joback Method
cpg	1733.24	J/molxK	1334.66	Joback Method
cpg	1790.21	J/molxK	1377.75	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=R135736&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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