

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

Inchi: InChI=1S/C27H26F14O4/c1-20-9-7-13(44-18(42)22(28,29)24(32,33)26(36,37)38)11-12(2
InchiKey: STYHDLOIJHHUKV-HNPOFBOPSA-N
Formula: C27H26F14O4
SMILES: C[C@]12CC=C(OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C=C1CCC1C2CC[C@@]2(C)C1CC[C@
Mol. weight [g/mol]: 680.47

Physical Properties

Property code	Value	Unit	Source
hfus	43.15	kJ/mol	Joback Method
log10ws	-9.71		Cheméo Relay (1.0)
logp	8.564		Crippen Method
mcvol	378.910	ml/mol	McGowan Method
tf	399.23	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1413.87	J/mol×K	987.87	Joback Method
cpg	1439.92	J/mol×K	1024.93	Joback Method
cpg	1467.43	J/mol×K	1061.99	Joback Method
cpg	1496.84	J/mol×K	1099.05	Joback Method
cpg	1528.60	J/mol×K	1136.10	Joback Method
cpg	1563.13	J/mol×K	1173.16	Joback Method
cpg	1600.88	J/mol×K	1210.22	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?Str2File=R135627>

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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