Testosterone, 3-chlorodifluoroacetate, 17«beta»-HFBate

Inchi: InChI=1S/C25H26ClF9O4/c1-20-9-7-13(38-19(37)23(26,29)30)11-12(20)3-4-14-15-5-6-1

InchiKey: KADFDSFRADELJP-FVLSIOMWSA-N

Formula: C25H26ClF9O4

SMILES: CC12CC=C(OC(=O)C(F)(F)Cl)C=C1CCC1C2CCC2(C)C(OC(=O)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 596.91

Physical Properties

Property code	Value	Unit	Source
gf	-1865.32	kJ/mol	Joback Method
hf	-2521.84	kJ/mol	Joback Method
hfus	41.59	kJ/mol	Joback Method
hvap	80.90	kJ/mol	Joback Method
log10ws	-8.95		Crippen Method
logp	7.562		Crippen Method
mcvol	354.120	ml/mol	McGowan Method
pc	988.26	kPa	Joback Method
rinpol	2591.00		NIST Webbook
rinpol	2591.00		NIST Webbook
tb	989.65	K	Joback Method
tc	1213.46	K	Joback Method
tf	680.78	K	Joback Method
vc	1.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1282.15	J/mol×K	989.65	Joback Method
cpg	1307.45	J/mol×K	1026.95	Joback Method
cpg	1334.09	J/mol×K	1064.25	Joback Method
cpg	1362.45	J/mol×K	1101.56	Joback Method
cpg	1392.92	J/mol×K	1138.86	Joback Method
cpg	1425.90	J/mol×K	1176.16	Joback Method
cpg	1461.78	J/mol×K	1213.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R135672&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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