

Testosterone, TFA

Inchi:	InChI=1S/C21H29F3O3/c1-19-9-7-13(25)11-12(19)3-4-14-15-5-6-17(27-18(26)21(22,23)
InchiKey:	RCYIQDXJWJPBOY-QBHRZVHSSA-N
Formula:	C21H29F3O3
SMILES:	CC12CCC(O)C=C1CCC1C2CCC2(C)C(OC(=O)C(F)(F)F)CCC12
Mol. weight [g/mol]:	386.45

Physical Properties

Property code	Value	Unit	Source
gf	-657.67	kJ/mol	Joback Method
hf	-1194.71	kJ/mol	Joback Method
hfus	32.34	kJ/mol	Joback Method
hvap	82.66	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	4.784		Crippen Method
mcvol	277.630	ml/mol	McGowan Method
pc	1531.86	kPa	Joback Method
rinsol	2352.00		NIST Webbook
tb	881.85	K	Joback Method
tc	1096.93	K	Joback Method
tf	566.12	K	Joback Method
vc	1.065	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1003.98	J/mol×K	881.85	Joback Method
cpg	1026.60	J/mol×K	917.70	Joback Method
cpg	1049.42	J/mol×K	953.54	Joback Method
cpg	1072.72	J/mol×K	989.39	Joback Method
cpg	1096.78	J/mol×K	1025.24	Joback Method
cpg	1121.87	J/mol×K	1061.09	Joback Method
cpg	1148.28	J/mol×K	1096.93	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R305376&Units=SI

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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