

Testosterone, 3-TFA, 17«beta»-Ac

Inchi:	InChI=1S/C23H29F3O4/c1-13(27)29-19-7-6-17-16-5-4-14-12-15(30-20(28)23(24,25)26)8
InchiKey:	PHVSTCDRRTYTLL-QTJPOHIASA-N
Formula:	C23H29F3O4
SMILES:	CC(=O)OC1CCC2C3CCC4=CC(OC(=O)C(F)(F)F)=CCC4(C)C3CCC12C
Mol. weight [g/mol]:	426.47

Physical Properties

Property code	Value	Unit	Source
gf	-709.89	kJ/mol	Joback Method
hf	-1261.91	kJ/mol	Joback Method
hfus	35.98	kJ/mol	Joback Method
hvap	80.86	kJ/mol	Joback Method
log10ws	-6.52		Crippen Method
logp	5.480		Crippen Method
mcvol	303.080	ml/mol	McGowan Method
pc	1332.96	kPa	Joback Method
rinpol	2520.00		NIST Webbook
rinpol	2520.00		NIST Webbook
tb	920.53	K	Joback Method
tc	1146.67	K	Joback Method
tf	617.52	K	Joback Method
vc	1.169	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1079.11	J/mol×K	920.53	Joback Method
cpg	1103.37	J/mol×K	958.22	Joback Method
cpg	1128.06	J/mol×K	995.91	Joback Method
cpg	1153.50	J/mol×K	1033.60	Joback Method
cpg	1180.01	J/mol×K	1071.29	Joback Method
cpg	1207.88	J/mol×K	1108.98	Joback Method
cpg	1237.44	J/mol×K	1146.67	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R135776&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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