

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

Inchi: InChI=1S/C23H29ClF2O4/c1-13(27)29-19-7-6-17-16-5-4-14-12-15(30-20(28)23(24,25)26

InchiKey: NTWLOFARRRXNBY-QTJPOHIASA-N

Formula: C23H29ClF2O4

SMILES: CC(=O)OC1CCC2C3CCC4=CC(OC(=O)C(F)(F)Cl)=CCC4(C)C3CCC12C

Mol. weight [g/mol]: 442.92

Physical Properties

Property code	Value	Unit	Source
gf	-527.01	kJ/mol	Joback Method
hf	-1081.54	kJ/mol	Joback Method
hfus	37.10	kJ/mol	Joback Method
hvap	86.06	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	5.750		Crippen Method
mcvol	313.550	ml/mol	McGowan Method
pc	1340.78	kPa	Joback Method
rinpol	2721.00		NIST Webbook
rinpol	2721.00		NIST Webbook
tb	958.69	K	Joback Method
tc	1194.41	K	Joback Method
tf	646.85	K	Joback Method
vc	1.200	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1105.00	J/mol×K	958.69	Joback Method
cpg	1130.64	J/mol×K	997.98	Joback Method
cpg	1157.13	J/mol×K	1037.26	Joback Method
cpg	1184.83	J/mol×K	1076.55	Joback Method
cpg	1214.09	J/mol×K	1115.84	Joback Method
cpg	1245.27	J/mol×K	1155.13	Joback Method
cpg	1278.71	J/mol×K	1194.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R135667&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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