Nortestosterone, HFB

Inchi: InChI=1S/C22H25F7O3/c1-19-9-8-14-13-5-3-12(30)10-11(13)2-4-15(14)16(19)6-7-17(19
InchiKey: BMBDDMGNZZCDHG-DVRUMADJSA-N
Formula: C22H25F7O3
SMILES: CC12CCC3C4CCC(=O)C=C4CCC3C1CCC2OC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 470.42

Physical Properties

Property code	Value	Unit	Source
gf	-1395.38	kJ/mol	Joback Method
hf	-1997.66	kJ/mol	Joback Method
hfus	33.07	kJ/mol	Joback Method
hvap	68.06	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	5.873		Crippen Method
mcvol	294.500	ml/mol	McGowan Method
pc	1220.85	kPa	Joback Method
rinpol	2440.00		NIST Webbook
rinpol	2440.00		NIST Webbook
tb	875.42	K	Joback Method
tc	1090.90	K	Joback Method
tf	572.33	K	Joback Method
vc	1.161	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1061.71	J/mol×K	875.42	Joback Method
cpg	1081.75	J/mol×K	911.33	Joback Method
cpg	1101.17	J/mol×K	947.25	Joback Method
cpg	1120.19	J/mol×K	983.16	Joback Method
cpg	1139.03	J/mol×K	1019.07	Joback Method
cpg	1157.91	J/mol×K	1054.98	Joback Method
cpg	1177.06	J/mol×K	1090.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R170006&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

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