Methyltestosterone, HFB

Inchi: InChI=1S/C24H29F7O3/c1-19-9-6-14(32)12-13(19)4-5-15-16(19)7-10-20(2)17(15)8-11-2
InchiKey: FXQFIJSPYKJFSH-XXYOTYRBSA-N
Formula: C24H29F7O3
SMILES: CC12CCC(=O)C=C1CCC1C2CCC2(C)C1CCC2(C)OC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 498.47

Physical Properties

Property code	Value	Unit	Source
gf	-1389.52	kJ/mol	Joback Method
hf	-2008.46	kJ/mol	Joback Method
hfus	25.65	kJ/mol	Joback Method
hvap	70.21	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	6.653		Crippen Method
mcvol	322.680	ml/mol	McGowan Method
pc	1138.27	kPa	Joback Method
rinpol	2272.00		NIST Webbook
tb	921.66	K	Joback Method
tc	1144.56	K	Joback Method
tf	642.67	K	Joback Method
vc	1.270	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1186.79	J/mol×K	921.66	Joback Method
cpg	1214.54	J/mol×K	958.81	Joback Method
cpg	1243.61	J/mol×K	995.96	Joback Method
cpg	1274.45	J/mol×K	1033.11	Joback Method
cpg	1307.49	J/mol×K	1070.26	Joback Method
cpg	1343.17	J/mol×K	1107.41	Joback Method
cpg	1381.93	J/mol×K	1144.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R169987&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