11«alpha»-Hydroxyprogesterone, TFA

Inchi: InChI=1S/C23H29F3O4/c1-12(27)16-6-7-17-15-5-4-13-10-14(28)8-9-21(13,2)19(15)18(1
InchiKey: FNZBZSOSILSBNO-SYAUZACASA-N
Formula: C23H29F3O4
SMILES: CC(=O)C1CCC2C3CCC4=CC(=O)CCC4(C)C3C(OC(=O)C(F)(F)F)CC12C
Mol. weight [g/mol]: 426.47

Physical Properties

Property code	Value	Unit	Source
gf	-755.52	kJ/mol	Joback Method
hf	-1334.04	kJ/mol	Joback Method
hfus	34.54	kJ/mol	Joback Method
hvap	81.43	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	4.808		Crippen Method
mcvol	303.080	ml/mol	McGowan Method
pc	1331.01	kPa	Joback Method
rinpol	2550.00		NIST Webbook
tb	957.12	K	Joback Method
tc	1191.79	K	Joback Method
tf	645.99	K	Joback Method
vc	1.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1123.95	J/mol×K	957.12	Joback Method
cpg	1149.89	J/mol×K	996.23	Joback Method
cpg	1176.37	J/mol×K	1035.34	Joback Method
cpg	1203.71	J/mol×K	1074.46	Joback Method
cpg	1232.24	J/mol×K	1113.57	Joback Method
cpg	1262.29	J/mol×K	1152.68	Joback Method
cpg	1294.18	J/mol×K	1191.79	Joback Method

Sources

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=R305118&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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