11«alpha»-hydroxyprogesterone, formate

Inchi: InChI=1S/C22H30O4/c1-13(24)17-6-7-18-16-5-4-14-10-15(25)8-9-21(14,2)20(16)19(26-1
InchiKey: OLKQKENKNWZZPM-UHFFFAOYSA-N
Formula: C22H30O4
SMILES: CC(=O)C1CCC2C3CCC4=CC(=O)CCC4(C)C3C(OC=O)CC12C
Mol. weight [g/mol]: 358.47

Physical Properties

Property code	Value	Unit	Source
gf	-152.95	kJ/mol	Joback Method
hf	-689.32	kJ/mol	Joback Method
hfus	30.81	kJ/mol	Joback Method
hvap	82.93	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.875		Crippen Method
mcvol	283.680	ml/mol	McGowan Method
pc	1577.21	kPa	Joback Method
rinpol	2536.00		NIST Webbook
tb	934.45	K	Joback Method
tc	1179.72	K	Joback Method
tf	622.60	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1036.96	J/mol×K	934.45	Joback Method
cpg	1063.64	J/mol×K	975.33	Joback Method
cpg	1090.69	J/mol×K	1016.21	Joback Method
cpg	1118.44	J/mol×K	1057.09	Joback Method
cpg	1147.22	J/mol×K	1097.96	Joback Method
cpg	1177.36	J/mol×K	1138.84	Joback Method
cpg	1209.20	J/mol×K	1179.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368390&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

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