11Beta,17alpha,21-trihydroxy-4-pregnene-3,20-dio

Other names: 17Alpha-hydroxycorticosterone
Inchi: InChI=1S/C21H30O5/c1-19-7-5-13(23)9-12(19)3-4-14-15-6-8-21(26,17(25)11-22)20(15,2
InchiKey: JYGXADMDTFJGBT-UHFFFAOYSA-N
Formula: C21H30O5
SMILES: CC12CCC(=O)C=C1CCC1C2C(O)CC2(C)C1CCC2(O)C(=O)CO
Mol. weight [g/mol]: 362.46
CAS: 116907-82-5

Physical Properties

Property code	Value	Unit	Source
gf	-372.80	kJ/mol	Joback Method
hf	-892.33	kJ/mol	Joback Method
hfus	30.71	kJ/mol	Joback Method
hvap	120.46	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	1.782		Crippen Method
mcvol	279.760	ml/mol	McGowan Method
pc	2147.32	kPa	Joback Method
tb	1117.27	K	Joback Method
tc	1367.94	K	Joback Method
tf	753.46	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1185.49	J/mol×K	1117.27	Joback Method
cpg	1228.38	J/mol×K	1159.05	Joback Method
cpg	1275.34	J/mol×K	1200.83	Joback Method
cpg	1326.87	J/mol×K	1242.60	Joback Method
cpg	1383.50	J/mol×K	1284.38	Joback Method
cpg	1445.75	J/mol×K	1326.16	Joback Method
cpg	1514.13	J/mol×K	1367.94	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=C116907825&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume