Pregn-4-ene-3,20-dione, 11«alpha»-hydroxy-, acetate

Other names: Pregn-4-ene-3,20-dione, 11-(acetyloxy)-, (11«alpha»)-
11«alpha»-Acetoxyprogesterone
11«alpha»-acetoxypregn-4-ene-3,20-dione
Progesterone, 11alpha-hydroxy-, acetate
11«alpha»-Hydroxyprogesterone Acetate
4-Pregnen-11«alpha»-ol-3,20-dione Acetate
3,20-Dioxopregn-4-en-11-yl acetate, (11«alpha»)-
11Alpha-acetoxypregn-4-ene-3,20-dione

Inchi: InChI=1S/C23H32O4/c1-13(24)18-7-8-19-17-6-5-15-11-16(26)9-10-22(15,3)21(17)20(27-

InchiKey: IWRPVTXREVYBHT-UHFFFAOYSA-N

Formula: C23H32O4

SMILES: CC(=O)OC1CC2(C)C(C(C)=O)CCC2C2CCC3=CC(=O)CCC3(C)C12

Mol. weight [g/mol]: 372.50

CAS: 2268-98-6

Physical Properties

Property code	Value	Unit	Source
gf	-173.93	kJ/mol	Joback Method
hf	-736.96	kJ/mol	Joback Method
hfus	32.71	kJ/mol	Joback Method
hvap	85.18	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.265		Crippen Method
mcvol	297.770	ml/mol	McGowan Method
pc	1451.25	kPa	Joback Method
tb	962.54	K	Joback Method
tc	1208.68	K	Joback Method
tf	641.80	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1104.24	J/mol×K	962.54	Joback Method

cpg	1132.17	J/mol×K	1003.56	Joback Method
cpg	1160.62	J/mol×K	1044.59	Joback Method
cpg	1189.90	J/mol×K	1085.61	Joback Method
cpg	1220.38	J/mol×K	1126.63	Joback Method
cpg	1252.37	J/mol×K	1167.66	Joback Method
cpg	1286.22	J/mol×K	1208.68	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=C2268986&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