

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

Other names:

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

U 0384

11 «alpha»-Hydroxyprogesterone

4-Pregnen-11 «alpha»-ol-3,20-dione

Progesterone, 11 «alpha»-hydroxy-

(11 «alpha»)-11-Hydroxypregn-4-ene-3,20-dione

11-«alpha»-hydroxypregn-4-ene-3,20-dione

Inchi: InChI=1S/C21H30O3/c1-12(22)16-6-7-17-15-5-4-13-10-14(23)8-9-20(13,2)19(15)18(24)1

InchiKey: BFZHCUBIASXHPK-FVCOPRDSSA-N

Formula: C21H30O3

SMILES: CC(=O)C1CCC2C3CCC4=CC(=O)CCC4(C)C3C(O)CC12C

Mol. weight [g/mol]: 330.46

CAS: 80-75-1

Physical Properties

Property code	Value	Unit	Source
gf	-93.67	kJ/mol	Joback Method
hf	-603.11	kJ/mol	Joback Method
hfus	28.83	kJ/mol	Joback Method
hvap	88.25	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	3.694		Crippen Method
mcvol	268.020	ml/mol	McGowan Method
pc	1755.07	kPa	Joback Method
rinpol	3104.00		NIST Webbook
rinpol	3336.70		NIST Webbook
rinpol	3336.70		NIST Webbook
tb	932.67	K	Joback Method
tc	1169.03	K	Joback Method
tf	607.92	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	993.63	J/mol×K	932.67	Joback Method
cpg	1019.24	J/mol×K	972.06	Joback Method
cpg	1045.37	J/mol×K	1011.46	Joback Method
cpg	1072.34	J/mol×K	1050.85	Joback Method
cpg	1100.47	J/mol×K	1090.24	Joback Method
cpg	1130.07	J/mol×K	1129.63	Joback Method
cpg	1161.46	J/mol×K	1169.03	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80751&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	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

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