

17«alpha»-Hydroxyprogesterone

Other names:	4-Pregnen-17«alpha»-ol-3,20-dione Pregn-4-ene-3,20-dione, 17-hydroxy-, (17«alpha»)- 17«alpha»-Hydroxyprogesterone 17-Hydroxypregn-4-ene-3,20-dione-, (17«alpha»)- 17alpha-Hydroxyprogesterone 17«alpha»-Hydroxypregna-4-ene-3,20-dione 17Alpha-hydroxypregna-4-ene-3,20-dione 17«alpha»-hydroxypregn-4-ene-3,20-dione
Inchi:	InChI=1S/C21H30O3/c1-13(22)21(24)11-8-18-16-5-4-14-12-15(23)6-9-19(14,2)17(16)7-1
InchiKey:	DBPWSSGDRRHUNT-WSBLSWJJSA-N
Formula:	C21H30O3
SMILES:	CC(=O)C1(O)CCC2C3CCC4=CC(=O)CCC4(C)C3CCC21C
Mol. weight [g/mol]:	330.46
CAS:	604-09-1

Physical Properties

Property code	Value	Unit	Source
gf	-91.45	kJ/mol	Joback Method
hf	-567.53	kJ/mol	Joback Method
hfus	21.46	kJ/mol	Joback Method
hvap	87.41	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	3.838		Crippen Method
mcvol	268.020	ml/mol	McGowan Method
pc	1875.65	kPa	Joback Method
tb	937.58	K	Joback Method
tc	1179.49	K	Joback Method
tf	636.06	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	991.36	J/molxK	937.58	Joback Method

cpg	1021.25	J/mol×K	977.90	Joback Method
cpg	1052.94	J/mol×K	1018.22	Joback Method
cpg	1086.89	J/mol×K	1058.54	Joback Method
cpg	1123.57	J/mol×K	1098.85	Joback Method
cpg	1163.45	J/mol×K	1139.17	Joback Method
cpg	1206.99	J/mol×K	1179.49	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=C604091&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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