Pregn-4-en-3-one, 20-hydroxy-, (20R)-

Other names: Pregn-4-en-3-one, 20«beta»-hydroxy-
Progesterol-20«beta»
20«beta»-Dihydroprogesterone
20«beta»-Hydroxydihydroprogesterone
20«beta»-Hydroxyprogesterone
20«beta»-Progerol
20-«beta»-Hydroxypregn-4-en-3-one
4-Pregnen-20«beta»-ol-3-one
20-Hydroxypregn-4-en-3-one, (20«beta»)-
(20R)-20-hydroxypregn-4-en-3-one

Inchi: InChI=1S/C21H32O2/c1-13(22)17-6-7-18-16-5-4-14-12-15(23)8-10-20(14,2)19(16)9-11-2

InchiKey: RWBRUCCWZPSBFC-WWRIRWJESA-N

Formula: C21H32O2

SMILES: CC(O)C1CCC2C3CCC4=CC(=O)CCC4(C)C3CCC12C

Mol. weight [g/mol]:   316.48

CAS: 145-15-3

Physical Properties

Property code	Value	Unit	Source
gf	40.52	kJ/mol	Joback Method
hf	-475.47	kJ/mol	Joback Method
hfus	22.64	kJ/mol	Joback Method
hvap	81.42	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.515		Crippen Method
mcvol	266.450	ml/mol	McGowan Method
pc	1723.16	kPa	Joback Method
tb	883.03	K	Joback Method
tc	1116.78	K	Joback Method
tf	547.23	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	964.98	J/mol×K	883.03	Joback Method
cpg	990.52	J/mol×K	921.99	Joback Method
cpg	1016.25	J/mol×K	960.95	Joback Method
cpg	1042.50	J/mol×K	999.91	Joback Method
cpg	1069.57	J/mol×K	1038.86	Joback Method
cpg	1097.78	J/mol×K	1077.82	Joback Method
cpg	1127.47	J/mol×K	1116.78	Joback Method

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C145153&Units=SI

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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