

3Beta-hydroxypregn-5-en-20-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:	QWVWXRKHAXWWSV-UHFFFAOYSA-N
Formula:	C21H32O2
SMILES:	CC(=O)C1CCC2C3CCC4=CC(O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	316.48
CAS:	566-66-5

Physical Properties

Property code	Value	Unit	Source
gf	28.92	kJ/mol	Joback Method
hf	-465.41	kJ/mol	Joback Method
hfus	29.32	kJ/mol	Joback Method
hvap	84.00	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.515		Crippen Method
mcvol	266.450	ml/mol	McGowan Method
pc	1704.71	kPa	Joback Method
tb	864.85	K	Joback Method
tc	1091.42	K	Joback Method
tf	539.70	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	949.54	J/molxK	864.85	Joback Method
cpg	974.02	J/molxK	902.61	Joback Method
cpg	998.64	J/molxK	940.37	Joback Method
cpg	1023.72	J/molxK	978.14	Joback Method
cpg	1049.57	J/molxK	1015.90	Joback Method
cpg	1076.50	J/molxK	1053.66	Joback Method
cpg	1104.85	J/molxK	1091.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C566665&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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