

17Alpha,21-dihydroxypregna-1,4-diene-3,20-dione

Inchi:	InChI=1S/C21H28O4/c1-19-8-5-14(23)11-13(19)3-4-15-16(19)6-9-20(2)17(15)7-10-21(20)
InchiKey:	BVAYTJBBDODANA-UHFFFAOYSA-N
Formula:	C21H28O4
SMILES:	CC12C=CC(=O)C=C1CCC1C2CCC2(C)C1CCC2(O)C(=O)CO
Mol. weight [g/mol]:	344.44
CAS:	1807-14-3

Physical Properties

Property code	Value	Unit	Source
gf	-198.31	kJ/mol	Joback Method
hf	-661.98	kJ/mol	Joback Method
hfus	26.77	kJ/mol	Joback Method
hvap	104.38	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	2.587		Crippen Method
mvol	269.590	ml/mol	McGowan Method
pc	2102.27	kPa	Joback Method
tb	1028.92	K	Joback Method
tc	1267.89	K	Joback Method
tf	697.64	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1048.66	J/molxK	1028.92	Joback Method
cpg	1082.34	J/molxK	1068.75	Joback Method
cpg	1118.88	J/molxK	1108.58	Joback Method
cpg	1158.75	J/molxK	1148.41	Joback Method
cpg	1202.40	J/molxK	1188.23	Joback Method
cpg	1250.29	J/molxK	1228.06	Joback Method
cpg	1302.87	J/molxK	1267.89	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=C1807143&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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