

5-«alpha»-Pregnane-17-«alpha»,20-«beta»,21-triol

Inchi:	InChI=1S/C21H36O3/c1-19-10-4-3-5-14(19)6-7-15-16(19)8-11-20(2)17(15)9-12-21(20,24)
InchiKey:	POBOSGNSIHOBXLX-AKFKKKQQA-N
Formula:	C21H36O3
SMILES:	CC12CCCCC1CCC1C2CCC2(C)C1CCC2(O)C(O)CO
Mol. weight [g/mol]:	336.51

Physical Properties

Property code	Value	Unit	Source
gf	-144.06	kJ/mol	Joback Method
hf	-693.64	kJ/mol	Joback Method
hfus	25.25	kJ/mol	Joback Method
hvap	108.12	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	3.504		Crippen Method
mcvol	280.920	ml/mol	McGowan Method
pc	1942.37	kPa	Joback Method
rinsol	2830.00		NIST Webbook
tb	991.00	K	Joback Method
tc	1215.12	K	Joback Method
tf	607.03	K	Joback Method
vc	1.042	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1121.54	J/molxK	991.00	Joback Method
cpg	1153.66	J/molxK	1028.35	Joback Method
cpg	1187.99	J/molxK	1065.71	Joback Method
cpg	1224.95	J/molxK	1103.06	Joback Method
cpg	1264.95	J/molxK	1140.41	Joback Method
cpg	1308.41	J/molxK	1177.76	Joback Method
cpg	1355.74	J/molxK	1215.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R149765&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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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