

3«alpha»,17«alpha»,21-trihydroxy-5«beta»-pregna

Inchi:	InChI=1S/C19H30O4/c20-10-18(22)19(23)8-7-16-15-3-1-11-9-12(21)2-4-13(11)14(15)5-6
InchiKey:	BVUYSJVBTLLMNN-CYBLYCBZSA-N
Formula:	C19H30O4
SMILES:	O=C(CO)C1(O)CCC2C3CCC4CC(O)CCC4C3CCC21
Mol. weight [g/mol]:	322.44

Physical Properties

Property code	Value	Unit	Source
gf	-284.11	kJ/mol	Joback Method
hf	-810.48	kJ/mol	Joback Method
hfus	38.85	kJ/mol	Joback Method
hvap	112.80	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	1.902		Crippen Method
mcvol	254.310	ml/mol	McGowan Method
pc	2173.43	kPa	Joback Method
rinqol	2845.00		NIST Webbook
tb	994.40	K	Joback Method
tc	1218.26	K	Joback Method
tf	597.38	K	Joback Method
vc	0.945	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1003.35	J/molxK	994.40	Joback Method
cpg	1023.65	J/molxK	1031.71	Joback Method
cpg	1044.03	J/molxK	1069.02	Joback Method
cpg	1064.68	J/molxK	1106.33	Joback Method
cpg	1085.83	J/molxK	1143.64	Joback Method
cpg	1107.67	J/molxK	1180.95	Joback Method
cpg	1130.42	J/molxK	1218.26	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=R248961&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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