Pregn-5-en-20-one, 3,17-dihydroxy-, (3«beta»)-

Other names:	Pregn-5-en-20-one, 3«beta»,17-dihydroxy- 17«alpha»-Hydroxypregnenolone 17-Hydroxy-«delta»5-pregnenolone 17-Hydroxypregnenolone 5-Pregnen-3«beta»,17«alpha»-diol-20-one 3-«beta»,17-Dihydroxypregn-5-en-20-one 3,17-Dihydroxypregn-5-en-20-one, (3«beta»,17«alpha»)- 3«beta»,17«alpha»-Dihydroxypregn-5-en-20-one NSC 63853
Inchi:	InChI=1S/C21H32O3/c1-13(22)21(24)11-8-18-16-5-4-14-12-15(23)6-9-19(14,2)17(16)7-1
InchiKey:	JERGUCIJOXJXHF-LRUBYMQBSA-N
Formula:	C21H32O3
SMILES:	CC(=O)C1(O)CCC2C3CC=C4CC(O)CCC4(C)C3CCC21C
Mol. weight [g/mol]:	332.48
CAS:	387-79-1

Physical Properties

Property code	Value	Unit	Source
gf	-113.39	kJ/mol	Joback Method
hf	-602.40	kJ/mol	Joback Method
hfus	27.11	kJ/mol	Joback Method
hvap	99.53	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	3.630		Crippen Method
mcvol	272.320	ml/mol	McGowan Method
pc	1915.26	kPa	Joback Method
rinpol	2889.90		NIST Webbook
tb	957.27	K	Joback Method
tc	1183.73	K	Joback Method
tf	624.42	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.15	J/mol×K	957.27	Joback Method
cpg	1060.55	J/mol×K	995.01	Joback Method
cpg	1091.88	J/mol×K	1032.76	Joback Method
cpg	1125.55	J/mol×K	1070.50	Joback Method
cpg	1161.97	J/mol×K	1108.24	Joback Method
cpg	1201.57	J/mol×K	1145.99	Joback Method
cpg	1244.75	J/mol×K	1183.73	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C387791&Units=SI
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

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
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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