5«beta»-Pregnan-3«beta»,20«alpha»-diol

Other names: 5B-Pregnan-3B,20A-diol
Inchi: InChI=1S/C21H36O2/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: YWYQTGBBEZQBGO-ZWMKSLNSSA-N
Formula: C21H36O2
SMILES: CC(O)C1CCC2C3CCC4CC(O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 320.51

Physical Properties

Property code	Value	Unit	Source
hfus	28.53	kJ/mol	Joback Method
log10ws	-4.83		Cheméo Relay (1.0)
logp	4.387		Crippen Method
mcvol	275.050	ml/mol	McGowan Method
tf	444.76	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1035.23	J/mol×K	893.91	Joback Method
cpg	1060.13	J/mol×K	929.77	Joback Method
cpg	1085.24	J/mol×K	965.63	Joback Method
cpg	1110.84	J/mol×K	1001.50	Joback Method
cpg	1137.20	J/mol×K	1037.36	Joback Method
cpg	1164.59	J/mol×K	1073.22	Joback Method
cpg	1193.29	J/mol×K	1109.08	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U126782&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point