

5-Pregnene-3«beta»,20«beta»,21-triol

Inchi:	InChI=1S/C21H34O3/c1-20-9-7-14(23)11-13(20)3-4-15-16-5-6-18(19(24)12-22)21(16,2)
InchiKey:	DAXILKUPMDAOAK-LVWWWKEUSA-N
Formula:	C21H34O3
SMILES:	CC12CCC(O)CC1=CCC1C2CCC2(C)C(C(O)CO)CCC12
Mol. weight [g/mol]:	334.49

Physical Properties

Property code	Value	Unit	Source
gf	-118.24	kJ/mol	Joback Method
hf	-662.57	kJ/mol	Joback Method
hfus	32.38	kJ/mol	Joback Method
hvap	110.23	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	3.280		Crippen Method
mcvol	276.620	ml/mol	McGowan Method
pc	1901.92	kPa	Joback Method
rinqol	2950.00		NIST Webbook
tb	994.90	K	Joback Method
tc	1218.95	K	Joback Method
tf	596.41	K	Joback Method
vc	1.030	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1083.83	J/molxK	994.90	Joback Method
cpg	1110.61	J/molxK	1032.24	Joback Method
cpg	1138.60	J/molxK	1069.58	Joback Method
cpg	1168.12	J/molxK	1106.93	Joback Method
cpg	1199.47	J/molxK	1144.27	Joback Method
cpg	1232.98	J/molxK	1181.61	Joback Method
cpg	1268.96	J/molxK	1218.95	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=R528886&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
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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