7-chloro-4-(dimethylamino)-1,6,10,11,12a-pentahy

Inchi: InChI=1S/C22H23ClN2O8/c1-21(32)7-6-8-15(25(2)3)17(28)13(20(24)31)19(30)22(8,33)1
InchiKey: DHPRQBPJLMKORJ-UHFFFAOYSA-N
Formula: C22H23ClN2O8
SMILES: CN(C)C1C(=O)C(C(N)=O)=C(O)C2(O)C(=O)C3=C(O)c4c(O)ccc(Cl)c4C(C)(O)C3CC12
Mol. weight [g/mol]: 478.88

Physical Properties

Property code	Value	Unit	Source
gf	-542.24	kJ/mol	Joback Method
hf	-1113.05	kJ/mol	Joback Method
hfus	59.71	kJ/mol	Joback Method
hvap	180.77	kJ/mol	Joback Method
log10ws	-2.94		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	0.282		Crippen Method
mcvol	322.160	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
tb	1543.06	K	Joback Method
tc	1999.69	K	Joback Method
tf	1210.36	K	Joback Method
vc	1.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1686.87	J/mol×K	1543.06	Joback Method
cpg	1833.67	J/mol×K	1619.16	Joback Method
cpg	2003.21	J/mol×K	1695.27	Joback Method
cpg	2197.81	J/mol×K	1771.37	Joback Method
cpg	2419.78	J/mol×K	1847.48	Joback Method
cpg	2671.46	J/mol×K	1923.58	Joback Method
cpg	2955.15	J/mol×K	1999.69	Joback Method

Sources

Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume