amikacin

Inchi: InChI=1S/C22H43N5O13/c23-2-1-8(29)20(36)27-7-3-6(25)18(39-22-16(34)15(33)13(31)9
InchiKey: LKCWBDHBTVXHDL-UHFFFAOYSA-N
Formula: C22H43N5O13
SMILES: NCCC(O)C(=O)NC1CC(N)C(OC2OC(CN)C(O)C(O)C2O)C(O)C1OC1OC(CO)C(O)C(N)C
Mol. weight [g/mol]: 585.61

Physical Properties

Property code	Value	Unit	Source
gf	-1137.78	kJ/mol	Joback Method
hf	-2254.04	kJ/mol	Joback Method
hfus	116.09	kJ/mol	Joback Method
hvap	264.77	kJ/mol	Joback Method
log10ws	-0.50		Aqueous Solubility Prediction Method
logp	-8.424		Crippen Method
mcvol	410.170	ml/mol	McGowan Method
pc	2235.52	kPa	Joback Method
tb	1935.27	K	Joback Method
tc	4390.44	K	Joback Method
tf	476.65	K	Aqueous Solubility Prediction Method
vc	1.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.42	J/mol×K	1935.27	Joback Method
cpg	36.40	J/mol×K	2344.46	Joback Method
cpg	-1391.74	J/mol×K	2753.66	Joback Method
cpg	-3311.74	J/mol×K	3162.85	Joback Method
cpg	-5749.35	J/mol×K	3572.05	Joback Method
cpg	-8730.33	J/mol×K	3981.24	Joback Method
cpg	-12280.42	J/mol×K	4390.44	Joback Method

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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