pimaricin

Inchi: InChI=1S/C33H47NO13/c1-18-10-8-6-4-3-5-7-9-11-21(45-32-30(39)28(34)29(38)19(2)44
InchiKey: NCXMLFZGDNKEPB-UHFFFAOYSA-N
Formula: C33H47NO13
SMILES: CC1CC=CC=CC=CC(OC2OC(C)C(O)C(N)C2O)CC2OC(O)(CC(O)CC3OC3C=CC(=
Mol. weight [g/mol]: 665.73

Physical Properties

Property code	Value	Unit	Source
gf	-1184.47	kJ/mol	Joback Method
hf	-2258.12	kJ/mol	Joback Method
hfus	102.03	kJ/mol	Joback Method
hvap	231.87	kJ/mol	Joback Method
log10ws	-3.21		Aqueous Solubility Prediction Method
logp	0.120		Crippen Method
mcvol	488.580	ml/mol	McGowan Method
pc	1306.12	kPa	Joback Method
tb	1902.20	K	Joback Method
tc	3017.66	K	Joback Method
tf	1136.13	K	Joback Method
vc	1.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1360.83	J/mol×K	1902.20	Joback Method
cpg	1008.69	J/mol×K	2088.11	Joback Method
cpg	570.68	J/mol×K	2274.02	Joback Method
cpg	47.41	J/mol×K	2459.93	Joback Method
cpg	-560.49	J/mol×K	2645.84	Joback Method
cpg	-1252.41	J/mol×K	2831.75	Joback Method
cpg	-2027.73	J/mol×K	3017.66	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