Digoxin (L1=41,8mg/mL, L2=68,2mg/mL, Z=40,1mg/mL)

Inchi: InChI=1S/C41H64O14/c1-19-36(47)28(42)15-34(50-19)54-38-21(3)52-35(17-30(38)44)55

InchiKey: LTMHDMANZUZIPE-UHFFFAOYSA-N

Formula: C41H64O14

SMILES: CC1OC(OC2C(O)CC(OC3C(O)CC(OC4CCC5(C)C(CCC6C5CC(O)C5(C)C(C7=CC(=O)C

Mol. weight [g/mol]: 780.95

Physical Properties

Property code	Value	Unit	Source
gf	-1112.62	kJ/mol	Joback Method
hf	-2553.86	kJ/mol	Joback Method
hfus	108.81	kJ/mol	Joback Method
hvap	231.99	kJ/mol	Joback Method
log10ws	-4.08		Estimated Solubility Method
log10ws	-4.12		Aqueous Solubility Prediction Method
logp	2.218		Crippen Method
mcvol	575.250	ml/mol	McGowan Method
pc	822.42	kPa	Joback Method
tb	1999.83	K	Joback Method
tc	3697.46	K	Joback Method
tf	1275.00	K	Joback Method
vc	2.086	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	4123.27	J/mol×K	1999.83	Joback Method
cpg	5342.13	J/mol×K	2282.77	Joback Method
cpg	7135.76	J/mol×K	2565.71	Joback Method
cpg	9646.31	J/mol×K	2848.64	Joback Method
cpg	13015.93	J/mol×K	3131.58	Joback Method
cpg	17386.79	J/mol×K	3414.52	Joback Method
cpg	22901.02	J/mol×K	3697.46	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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