4-(3,14-dihydroxy-10,13-dimethyl-1,2,3,4,5,6,7,8,9,

Inchi: InChI=1S/C23H34O4/c1-21-8-5-16(24)12-15(21)3-4-19-18(21)6-9-22(2)17(7-10-23(19,22
InchiKey: XZTUSOXSLKTKJQ-UHFFFAOYSA-N
Formula: C23H34O4
SMILES: CC12CCC(O)CC1CCC1C2CCC2(C)C(C3=CC(=O)OC3)CCC12O
Mol. weight [g/mol]: 374.52

Physical Properties

Property code	Value	Unit	Source
gf	-139.79	kJ/mol	Joback Method
hf	-740.32	kJ/mol	Joback Method
hfus	32.12	kJ/mol	Joback Method
hvap	106.25	kJ/mol	Joback Method
log10ws	-4.57		Aqueous Solubility Prediction Method
logp	3.604		Crippen Method
mcvol	295.510	ml/mol	McGowan Method
pc	1835.69	kPa	Joback Method
tb	1059.21	K	Joback Method
tc	1305.01	K	Joback Method
tf	702.72	K	Joback Method
vc	1.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1232.94	J/mol×K	1059.21	Joback Method
cpg	1272.17	J/mol×K	1100.18	Joback Method
cpg	1314.50	J/mol×K	1141.14	Joback Method
cpg	1360.42	J/mol×K	1182.11	Joback Method
cpg	1410.47	J/mol×K	1223.07	Joback Method
cpg	1465.14	J/mol×K	1264.04	Joback Method
cpg	1524.94	J/mol×K	1305.01	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