Dihydroisovaltrate

Other names: Dihydroisovaltrate
Inchi: InChI=1S/C22H32O8/c1-12(2)6-18(24)26-9-15-10-27-21(30-19(25)7-13(3)4)20-16(15)8-1
InchiKey: PHHROXLDZHUIGO-UHFFFAOYSA-N
Formula: C22H32O8
SMILES: CC(=O)OC1CC2C(COC(=O)CC(C)C)=COC(OC(=O)CC(C)C)C2C12CO2
Mol. weight [g/mol]: 424.49

Physical Properties

Property code	Value	Unit	Source
hfus	56.89	kJ/mol	Joback Method
logp	2.742		Crippen Method
mcvol	318.020	ml/mol	McGowan Method
rinpol	2545.70		NIST Webbook
rinpol	2545.70		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1150.61	J/mol×K	1008.45	Joback Method
cpg	1170.80	J/mol×K	1046.61	Joback Method
cpg	1190.70	J/mol×K	1084.78	Joback Method
cpg	1210.45	J/mol×K	1122.94	Joback Method
cpg	1230.24	J/mol×K	1161.10	Joback Method
cpg	1250.23	J/mol×K	1199.26	Joback Method
cpg	1270.59	J/mol×K	1237.43	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18296452&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity

hfus: Enthalpy of fusion at standard conditions

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices