didrovaltrate

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]: 424.48
CAS: 18296-45-2

Physical Properties

Property code	Value	Unit	Source
gf	-587.05	kJ/mol	Joback Method
hf	-1279.42	kJ/mol	Joback Method
hfus	56.89	kJ/mol	Joback Method
hvap	99.55	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	2.742		Crippen Method
mcvol	318.020	ml/mol	McGowan Method
pc	1318.48	kPa	Joback Method
rinpol	2545.70		NIST Webbook
rinpol	2545.70		NIST Webbook
tb	1008.45	K	Joback Method
tc	1237.43	K	Joback Method
tf	652.80	K	Joback Method
vc	1.206	m3/kmol	Joback Method

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18296452&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume