Homodihydroisovaltrate

Inchi: InChI=1S/C23H34O8/c1-6-14(4)8-20(26)31-22-21-17(9-18(30-15(5)24)23(21)12-29-23)1
InchiKey: NQYKVDKWBKOHRD-UHFFFAOYSA-N
Formula: C23H34O8
SMILES: CCC(C)CC(=O)OC1OC=C(COC(=O)CC(C)C)C2CC(OC(C)=O)C3(CO3)C12
Mol. weight [g/mol]: 438.51
CAS: 18361-41-6

Physical Properties

Property code	Value	Unit	Source
gf	-578.63	kJ/mol	Joback Method
hf	-1300.06	kJ/mol	Joback Method
hfus	59.48	kJ/mol	Joback Method
hvap	101.77	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.132		Crippen Method
mcvol	332.110	ml/mol	McGowan Method
pc	1231.15	kPa	Joback Method
rinpol	2648.40		NIST Webbook
rinpol	2648.40		NIST Webbook
tb	1031.33	K	Joback Method
tc	1263.54	K	Joback Method
tf	664.07	K	Joback Method
vc	1.262	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1215.02	J/mol×K	1031.33	Joback Method
cpg	1236.07	J/mol×K	1070.03	Joback Method
cpg	1256.87	J/mol×K	1108.73	Joback Method
cpg	1277.59	J/mol×K	1147.43	Joback Method
cpg	1298.42	J/mol×K	1186.13	Joback Method
cpg	1319.52	J/mol×K	1224.83	Joback Method
cpg	1341.09	J/mol×K	1263.54	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18361416&Units=SI

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