[4-(5-Hydroxy-2,4-dimethoxyphenyl)-3-methoxyca
acid, methyl ester

Inchi: InChI=1S/C20H26O8/c1-25-13-9-15(22)20(16(10-13)26-2)19-12(8-18(24)28-4)5-11(6-14

InchiKey: YIFWAUXYLIDRDO-UHFFFAOYSA-N

Formula: C20H26O8

SMILES: COC(=O)CC1CC(=O)C(c2c(O)cc(OC)cc2OC)C(CC(=O)OC)C1

Mol. weight [g/mol]: 394.42

Physical Properties

Property code	Value	Unit	Source
gf	-735.35	kJ/mol	Joback Method
hf	-1297.95	kJ/mol	Joback Method
hfus	48.04	kJ/mol	Joback Method
hvap	103.92	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.215		Crippen Method
mcvol	292.100	ml/mol	McGowan Method
pc	1657.84	kPa	Joback Method
rinpol	2979.00		NIST Webbook
rinpol	2979.00		NIST Webbook
tb	1049.71	K	Joback Method
tc	1291.32	K	Joback Method
tf	734.24	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1013.98	J/mol×K	1049.71	Joback Method
cpg	1024.12	J/mol×K	1089.98	Joback Method
cpg	1032.11	J/mol×K	1130.25	Joback Method
cpg	1037.92	J/mol×K	1170.51	Joback Method
cpg	1041.54	J/mol×K	1210.78	Joback Method
cpg	1042.93	J/mol×K	1251.05	Joback Method
cpg	1042.08	J/mol×K	1291.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R635122&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