Acetophenone, 4-hydroxy-3,5-dimethoxy, O-methyloxime

Inchi: InChI=1S/C11H15NO4/c1-7(12-16-4)8-5-9(14-2)11(13)10(6-8)15-3/h5-6,13H,1-4H3

InchiKey: GWRCWEKFIJBHPQ-UHFFFAOYSA-N

Formula: C11H15NO4

SMILES: CON=C(C)c1cc(OC)c(O)c(OC)c1

Mol. weight [g/mol]: 225.24

Physical Properties

Property code	Value	Unit	Source
hf	-558.32	kJ/mol	Joback Method
hvap	67.32	kJ/mol	Joback Method
log10ws	-1.82		Crippen Method
logp	1.780		Crippen Method
mcvol	171.250	ml/mol	McGowan Method
pc	2563.69	kPa	Joback Method
rinpol	1842.00		NIST Webbook
tb	712.16	K	Joback Method
tc	938.57	K	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=R99905&Units=SI

Legend

hf: Enthalpy of formation 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