Benzaldehyde, 3,4-dihydroxy, O-methyloxime

Inchi: InChI=1S/C8H9NO3/c1-12-9-5-6-2-3-7(10)8(11)4-6/h2-5,10-11H,1H3

InchiKey: QKIMWRSLZXAMIW-UHFFFAOYSA-N

Formula: C8H9NO3

SMILES: CON=Cc1ccc(O)c(O)c1

Mol. weight [g/mol]:   167.16

Physical Properties

Property code	Value	Unit	Source
hf	-376.54	kJ/mol	Joback Method
hvap	67.43	kJ/mol	Joback Method
log10ws	-0.71		Crippen Method
logp	1.078		Crippen Method
mcvol	123.110	ml/mol	McGowan Method
pc	4571.55	kPa	Joback Method
rinpol	1704.00		NIST Webbook
tb	669.46	K	Joback Method
tc	919.36	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R100022&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

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