Benzaldehyde, 3-hydroxy-4-methoxy, O-methyloxime

Inchi: InChI=1S/C9H11NO3/c1-12-9-4-3-7(5-8(9)11)6-10-13-2/h3-6,11H,1-2H3/b10-6+

InchiKey: LLQDRFKTWYEAKV-UXBLZVDNSA-N

Formula: C9H11NO3

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

Mol. weight [g/mol]: 181.19

Physical Properties

Property code	Value	Unit	Source
hf	-363.56	kJ/mol	Joback Method
hvap	59.71	kJ/mol	Joback Method
log10ws	-1.29		Crippen Method
logp	1.381		Crippen Method
mcvol	137.200	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
rinpol	1623.00		NIST Webbook
tb	639.12	K	Joback Method
tc	872.83	K	Joback Method

Sources

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=R100042&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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