

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

Inchi:	InChI=1S/C9H11NO3/c1-12-9-5-7(6-10-13-2)3-4-8(9)11/h3-6,11H,1-2H3/b10-6+
InchiKey:	TWLUCZWNLUUHJT-UXBLZVDNSA-N
Formula:	C9H11NO3
SMILES:	CON=Cc1ccc(O)c(OC)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	1624.00		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=R100106&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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

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