Benzaldehyde, 3,4-methylenedioxy, methoxime

Inchi: InChI=1S/C9H9NO3/c1-11-10-5-7-2-3-8-9(4-7)13-6-12-8/h2-5H,6H2,1H3
InchiKey: ABHAGWDDCROTGV-UHFFFAOYSA-N
Formula: C9H9NO3
SMILES: CON=Cc1ccc2c(c1)OCO2
Mol. weight [g/mol]: 179.17

Physical Properties

Property code	Value	Unit	Source
hf	-236.36	kJ/mol	Joback Method
hvap	54.19	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.396		Crippen Method
mcvol	126.340	ml/mol	McGowan Method
pc	3235.66	kPa	Joback Method
rinpol	1419.00		NIST Webbook
tb	606.37	K	Joback Method
tc	845.84	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=R92545&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