

Benzaldehyde, 4-hydroxy, O-methyloxime

Inchi: InChI=1S/C8H9NO2/c1-11-9-6-7-2-4-8(10)5-3-7/h2-6,10H,1H3/b9-6+
InchiKey: DAJIRPMNQQGGJN-RMKNXTFCSA-N
Formula: C8H9NO2
SMILES: CON=Cc1ccc(O)cc1
Mol. weight [g/mol]: 151.16

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | -199.23 | kJ/mol | Joback Method |
| hvap | 54.42 | kJ/mol | Joback Method |
| log10ws | -1.17 | | Crippen Method |
| logp | 1.373 | | Crippen Method |
| mcvol | 117.240 | ml/mol | McGowan Method |
| pc | 3773.04 | kPa | Joback Method |
| rinpol | 1475.00 | | NIST Webbook |
| tb | 588.84 | K | Joback Method |
| tc | 830.11 | 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=R100126&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 |
| rinpola: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |

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