# Benzaldehyde, 3,4-dimethoxy-

| | |
|---|---|
| **Other names:** | 3,4-Dimethoxybenzaldehyde |
| | 3,4-Dimethoxybenzenecarbonal |
| | 4-O-Methylvanillin |
| | Benzaldehyde, 3,4-dimethoxy-veratraldehyde |
| | Methylvanillin |
| | NSC 24521 |
| | Protocatechualdehyde dimethyl ether |
| | Protocatechuecaldehyde dimethyl ether |
| | Protocatechuic aldehyde dimethyl ether |
| | Vanillin methyl ether |
| | Veratral |
| | Veratraldehyde |
| | Veratric aldehyde |
| | Veratrum aldehyde |
| | Veratryl aldehyde |
| | p-Veratric aldehyde |
| **Inchi:** | InChI=1S/C9H10O3/c1-11-8-4-3-7(6-10)5-9(8)12-2/h3-6H,1-2H3 |
| **InchiKey:** | WJUFSDZVCOTFON-UHFFFAOYSA-N |
| **Formula:** | C9H10O3 |
| **SMILES:** | COc1ccc(C=O)cc1OC |
| **Mol. weight [g/mol]:** | 166.17 |
| **CAS:** | 120-14-9 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -191.47 | kJ/mol | Joback Method |
| hf | -365.52 | kJ/mol | Joback Method |
| hfus | 16.99 | kJ/mol | Joback Method |
| hvap | 50.77 | kJ/mol | Joback Method |
| log10ws | -1.16 | | Aqueous Solubility Prediction Method |
| logp | 1.516 | | Crippen Method |
| mcvol | 127.220 | ml/mol | McGowan Method |
| pc | 3299.15 | kPa | Joback Method |
| rinpol | 1427.00 | | NIST Webbook |
| rinpol | 1427.00 | | NIST Webbook |
| rinpol | 1425.00 | | NIST Webbook |

| | | | |
|---|---|---|---|
| rinpol | 1422.00 | | NIST Webbook |
| rinpol | 1422.00 | | NIST Webbook |
| rinpol | 1423.00 | | NIST Webbook |
| rinpol | 1422.00 | | NIST Webbook |
| rinpol | 1427.00 | | NIST Webbook |
| rinpol | 1419.00 | | NIST Webbook |
| rinpol | 1423.00 | | NIST Webbook |
| ripol | 2409.00 | | NIST Webbook |
| ripol | 2417.00 | | NIST Webbook |
| ripol | 2400.00 | | NIST Webbook |
| ripol | 2420.00 | | NIST Webbook |
| ripol | 2417.00 | | NIST Webbook |
| ripol | 2405.00 | | NIST Webbook |
| tb | 554.20 | K | NIST Webbook |
| tc | 746.40 | K | Joback Method |
| tf | 316.65 | K | Aqueous Solubility Prediction Method |
| vc | 0.484 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 279.82 | J/mol×K | 535.46 | Joback Method |
| cpg | 291.21 | J/mol×K | 570.62 | Joback Method |
| cpg | 302.11 | J/mol×K | 605.77 | Joback Method |
| cpg | 312.49 | J/mol×K | 640.93 | Joback Method |
| cpg | 322.35 | J/mol×K | 676.09 | Joback Method |
| cpg | 331.68 | J/mol×K | 711.24 | Joback Method |
| cpg | 340.46 | J/mol×K | 746.40 | Joback Method |
| dvisc | 0.0011750 | Pa×s | 329.11 | Joback Method |
| dvisc | 0.0007578 | Pa×s | 363.50 | Joback Method |
| dvisc | 0.0005273 | Pa×s | 397.89 | Joback Method |
| dvisc | 0.0003887 | Pa×s | 432.29 | Joback Method |
| dvisc | 0.0002996 | Pa×s | 466.68 | Joback Method |
| dvisc | 0.0002394 | Pa×s | 501.07 | Joback Method |
| dvisc | 0.0001969 | Pa×s | 535.46 | Joback Method |
| hfust | 20.30 | kJ/mol | 317.00 | NIST Webbook |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 446.70 | K | 2.40 | NIST Webbook |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C120149&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Joback Method:** https://en.wikipedia.org/wiki/Joback_method
**Aqueous Solubility Prediction Method:** http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

# Legend

**cpg:** Ideal gas heat capacity
**dvisc:** Dynamic viscosity
**gf:** Standard Gibbs free energy of formation
**hf:** Enthalpy of formation at standard conditions
**hfus:** Enthalpy of fusion at standard conditions
**hfust:** Enthalpy of fusion at a given temperature
**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
**ripol:** Polar retention indices
**tb:** Normal Boiling Point Temperature
**tbrp:** Boiling point at reduced pressure
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point
**vc:** Critical Volume

Latest version available from: