# Benzaldehyde, 3,4,5-trimethoxy-

**Other names:** 3,4,5-Trimethoxybenzaldehyde
**Inchi:** InChI=1S/C10H12O4/c1-12-8-4-7(6-11)5-9(13-2)10(8)14-3/h4-6H,1-3H3
**InchiKey:** OPHQOIGEOHXOGX-UHFFFAOYSA-N
**Formula:** C10H12O4
**SMILES:** COc1cc(C=O)cc(OC)c1OC
**Mol. weight [g/mol]:** 196.20
**CAS:** 86-81-7

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -297.68 | kJ/mol | Joback Method |
| hf | -529.85 | kJ/mol | Joback Method |
| hfus | 20.38 | kJ/mol | Joback Method |
| hvap | 56.07 | kJ/mol | Joback Method |
| log10ws | -2.07 | | Crippen Method |
| logp | 1.525 | | Crippen Method |
| mcvol | 147.180 | ml/mol | McGowan Method |
| pc | 2862.74 | kPa | Joback Method |
| rinpol | 1608.00 | | NIST Webbook |
| rinpol | 1551.00 | | NIST Webbook |
| rinpol | 1621.00 | | NIST Webbook |
| ripol | 2539.00 | | NIST Webbook |
| tb | 585.74 | K | Joback Method |
| tc | 792.23 | K | Joback Method |
| tf | 375.13 | K | Joback Method |
| vc | 0.558 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 347.43 | J/mol×K | 585.74 | Joback Method |
| cpg | 402.61 | J/mol×K | 757.82 | Joback Method |
| cpg | 392.68 | J/mol×K | 723.40 | Joback Method |
| cpg | 382.17 | J/mol×K | 688.99 | Joback Method |

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|---|---|---|---|---|
| cpg | 371.11 | J/mol×K | 654.57 | Joback Method |
| cpg | 359.52 | J/mol×K | 620.16 | Joback Method |
| cpg | 411.94 | J/mol×K | 792.23 | Joback Method |
| dvisc | 0.0001477 | Pa×s | 585.74 | Joback Method |
| dvisc | 0.0001775 | Pa×s | 550.64 | Joback Method |
| dvisc | 0.0002187 | Pa×s | 515.54 | Joback Method |
| dvisc | 0.0002780 | Pa×s | 480.44 | Joback Method |
| dvisc | 0.0003668 | Pa×s | 445.33 | Joback Method |
| dvisc | 0.0005076 | Pa×s | 410.23 | Joback Method |
| dvisc | 0.0007464 | Pa×s | 375.13 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 437.20 | K | 1.30 | NIST Webbook |

# 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=C86817&Units=SI

# 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
**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 |