# 2,4,6-Trimethoxybenzaldehyde

**Other names:** Benzaldehyde, 2,4,6-trimethoxy-
**Inchi:** InChI=1S/C10H12O4/c1-12-7-4-9(13-2)8(6-11)10(5-7)14-3/h4-6H,1-3H3
**InchiKey:** CRBZVDLXAIFERF-UHFFFAOYSA-N
**Formula:** C10H12O4
**SMILES:** COc1cc(OC)c(C=O)c(OC)c1
**Mol. weight [g/mol]:** 196.20
**CAS:** 830-79-5

## 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 |
| 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 | 359.52 | J/mol×K | 620.16 | Joback Method |
| cpg | 371.11 | J/mol×K | 654.57 | Joback Method |
| cpg | 382.17 | J/mol×K | 688.99 | Joback Method |
| cpg | 392.68 | J/mol×K | 723.40 | Joback Method |
| cpg | 402.61 | J/mol×K | 757.82 | Joback Method |
| cpg | 411.94 | J/mol×K | 792.23 | Joback Method |
| dvisc | 0.0007464 | Pa×s | 375.13 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0005076 | Pa×s | 410.23 | Joback Method |
| dvisc | 0.0003668 | Pa×s | 445.33 | Joback Method |
| dvisc | 0.0002780 | Pa×s | 480.44 | Joback Method |
| dvisc | 0.0002187 | Pa×s | 515.54 | Joback Method |
| dvisc | 0.0001775 | Pa×s | 550.64 | Joback Method |
| dvisc | 0.0001477 | Pa×s | 585.74 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C830795&Units=SI |
| **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 |

# Legend

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|---|---|
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |