# 2,3-DIMETHOXYBENZOIC ACID

**Other names:** Benzoic acid, 2,3-dimethoxy-
o-Veratric acid
**Inchi:** InChI=1S/C9H10O4/c1-12-7-5-3-4-6(9(10)11)8(7)13-2/h3-5H,1-2H3,(H,10,11)
**InchiKey:** FODBVCSYJKNBLO-UHFFFAOYSA-N
**Formula:** C9H10O4
**SMILES:** COc1cccc(C(=O)O)c1OC
**Mol. weight [g/mol]:** 182.18

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -4283.80 ± 0.80 | kJ/mol | NIST Webbook |
| hf | -574.94 | kJ/mol | Cheméo Relay (1.0) |
| hfs | -687.00 ± 1.40 | kJ/mol | NIST Webbook |
| hfus | 20.39 | kJ/mol | Joback Method |
| hsub | 116.60 ± 0.30 | kJ/mol | NIST Webbook |
| hsub | 116.60 ± 0.30 | kJ/mol | NIST Webbook |
| hvap | 95.57 | kJ/mol | Cheméo Relay (1.0) |
| ie | 8.51 | eV | Cheméo Relay (1.0) |
| log10ws | -2.14 | | Aqueous Solubility Prediction Method |
| logp | 1.402 | | Crippen Method |
| mcvol | 133.090 | ml/mol | McGowan Method |
| rinpol | 1414.00 | | NIST Webbook |
| rinpol | 1414.00 | | NIST Webbook |
| tb | 571.85 | K | Cheméo Relay (1.0) |
| tc | 794.37 | K | Cheméo Relay (1.0) |
| tf | 417.72 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 324.57 | J/mol×K | 632.85 | Joback Method |
| cpg | 376.13 | J/mol×K | 834.15 | Joback Method |
| cpg | 368.87 | J/mol×K | 800.60 | Joback Method |

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|---|---|---|---|---|
| cpg | 361.07 | J/mol×K | 767.05 | Joback Method |
| cpg | 352.73 | J/mol×K | 733.50 | Joback Method |
| cpg | 343.86 | J/mol×K | 699.95 | Joback Method |
| cpg | 334.47 | J/mol×K | 666.40 | Joback Method |
| dvisc | 0.0001872 | Pa×s | 515.36 | Joback Method |
| dvisc | 0.0000571 | Pa×s | 632.85 | Joback Method |
| dvisc | 0.0000805 | Pa×s | 593.69 | Joback Method |
| dvisc | 0.0001191 | Pa×s | 554.52 | Joback Method |
| dvisc | 0.0012398 | Pa×s | 397.86 | Joback Method |
| dvisc | 0.0003170 | Pa×s | 476.19 | Joback Method |
| dvisc | 0.0005897 | Pa×s | 437.03 | Joback Method |
| hsubt | 115.10 ± 0.30 | kJ/mol | 346.00 | NIST Webbook |

# Sources

**Cheméo Relay (1.0):**

**Cheméo Relay (1.0, beta):**

**Aqueous Solubility Prediction Method:** http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C1521386&Units=SI

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# Legend

**chs:** Standard solid enthalpy of combustion
**cpg:** Ideal gas heat capacity
**dvisc:** Dynamic viscosity
**hf:** Enthalpy of formation at standard conditions
**hfs:** Solid phase enthalpy of formation at standard conditions
**hfus:** Enthalpy of fusion at standard conditions
**hsub:** Enthalpy of sublimation at standard conditions
**hsubt:** Enthalpy of sublimation at a given temperature
**hvap:** Enthalpy of vaporization at standard conditions
**ie:** Ionization energy
**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume

| | |
|---|---|
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |