# ETHYL 3-HYDROXYBENZOATE

**Other names:** 3-hydroxybenzoic acid ethyl ester
benzoic acid, 3-hydroxy-, ethyl ester
benzoic acid, m-hydroxy-, ethyl ester
ethyl m-hydroxybenzoate
m-Hydroxybenzoic acid ethyl ester
m-ethoxycarbonylphenol

**Inchi:** InChI=1S/C9H10O3/c1-2-12-9(11)7-4-3-5-8(10)6-7/h3-6,10H,2H2,1H3

**InchiKey:** MWSMNBYIEBRXAL-UHFFFAOYSA-N

**Formula:** C9H10O3

**SMILES:** CCOC(=O)c1cccc(O)c1

**Mol. weight [g/mol]:** 166.18

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.6390 | | Cheméo Relay (1.0) |
| gf | -251.23 | kJ/mol | Joback Method |
| hf | -485.21 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 21.68 | kJ/mol | Joback Method |
| hvap | 79.73 | kJ/mol | Cheméo Relay (1.0) |
| ie | 8.67 | eV | Cheméo Relay (1.0) |
| log10ws | -1.82 | | Cheméo Relay (1.0) |
| logp | 1.569 | | Crippen Method |
| mcvol | 127.220 | ml/mol | McGowan Method |
| pc | 4130.29 | kPa | Joback Method |
| tb | 568.20 | K | NIST Webbook |
| tc | 748.52 | K | Cheméo Relay (1.0) |
| tf | 343.84 | K | Cheméo Relay (1.0) |
| vc | 0.455 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 304.03 | J/mol×K | 588.91 | Joback Method |
| cpg | 361.35 | J/mol×K | 816.64 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 353.29 | J/mol×K | 778.68 | Joback Method |
| cpg | 344.71 | J/mol×K | 740.73 | Joback Method |
| cpg | 335.56 | J/mol×K | 702.77 | Joback Method |
| cpg | 325.77 | J/mol×K | 664.82 | Joback Method |
| cpg | 315.28 | J/mol×K | 626.86 | Joback Method |
| dvisc | 0.0001481 | Pa×s | 495.20 | Joback Method |
| dvisc | 0.0000400 | Pa×s | 588.91 | Joback Method |
| dvisc | 0.0000590 | Pa×s | 557.67 | Joback Method |
| dvisc | 0.0000909 | Pa×s | 526.44 | Joback Method |
| dvisc | 0.0010100 | Pa×s | 401.49 | Joback Method |
| dvisc | 0.0002577 | Pa×s | 463.96 | Joback Method |
| dvisc | 0.0004856 | Pa×s | 432.73 | Joback Method |
| hvapt | 78.40 | kJ/mol | 360.00 | Gas-phase enthalpies of formation of ethyl hydroxybenzoates: An experimental and theoretical approach |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 460.70 | K | 4.10 | NIST Webbook |
| tbrp | 484.20 | K | 8.70 | NIST Webbook |

# Sources

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

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

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**Cheméo Relay (1.0):**

**Cheméo Relay (1.0, beta):**

**Gas-phase enthalpies of formation of ethyl hydroxybenzoates: An experimental and theoretical approach:** https://www.doi.org/10.1016/j.jct.2017.09.007

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C7781988&Units=SI

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

# Legend

| | |
|---|---|
| **af:** | Acentric Factor |
| **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 |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **ie:** | Ionization energy |
| **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 |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |