# 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]:** | 166.17 |
| **CAS:** | 7781-98-8 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -251.23 | kJ/mol | Joback Method |
| hf | -414.67 | kJ/mol | Joback Method |
| hfus | 21.68 | kJ/mol | Joback Method |
| hvap | 60.07 | kJ/mol | Joback Method |
| log10ws | -1.68 | | Crippen Method |
| 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 | 816.64 | K | Joback Method |
| tf | 401.49 | K | Joback Method |
| vc | 0.421 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| 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 |
| cpg | 304.03 | J/mol×K | 588.91 | Joback Method |
| dvisc | 0.0010100 | Pa×s | 401.49 | 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 | 0.0001481 | Pa×s | 495.20 | 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

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

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

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

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

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

**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 |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **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 |