# Ethyl-3-methoxybenzoate

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|---|---|
| **Other names:** | ethyl m-anisate |
| | Benzoic acid, 3-methoxy-, ethyl ester |
| **Inchi:** | InChI=1S/C10H12O3/c1-3-13-10(11)8-5-4-6-9(7-8)12-2/h4-7H,3H2,1-2H3 |
| **InchiKey:** | GSQLMBQLTPEPHD-UHFFFAOYSA-N |
| **Formula:** | C10H12O3 |
| **SMILES:** | CCOC(=O)c1cccc(OC)c1 |
| **Mol. weight [g/mol]:** | 180.20 |
| **CAS:** | 10259-22-0 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -202.82 | kJ/mol | Joback Method |
| hf | -401.69 | kJ/mol | Joback Method |
| hfus | 19.28 | kJ/mol | Joback Method |
| hvap | 52.36 | kJ/mol | Joback Method |
| log10ws | -2.25 | | Crippen Method |
| logp | 1.872 | | Crippen Method |
| mcvol | 141.310 | ml/mol | McGowan Method |
| pc | 2976.29 | kPa | Joback Method |
| rinpol | 1424.00 | | NIST Webbook |
| tb | 533.65 ± 1.00 | K | NIST Webbook |
| tc | 770.06 | K | Joback Method |
| tf | 335.79 | K | Joback Method |
| vc | 0.529 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 323.98 | J/mol×K | 558.57 | Joback Method |
| cpg | 382.66 | J/mol×K | 734.81 | Joback Method |
| cpg | 372.24 | J/mol×K | 699.56 | Joback Method |
| cpg | 361.16 | J/mol×K | 664.31 | Joback Method |
| cpg | 349.42 | J/mol×K | 629.07 | Joback Method |
| cpg | 337.02 | J/mol×K | 593.82 | Joback Method |

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|---|---|---|---|---|
| cpg | 392.43 | J/mol×K | 770.06 | Joback Method |
| dvisc | 0.0001728 | Pa×s | 558.57 | Joback Method |
| dvisc | 0.0002153 | Pa×s | 521.44 | Joback Method |
| dvisc | 0.0002774 | Pa×s | 484.31 | Joback Method |
| dvisc | 0.0003728 | Pa×s | 447.18 | Joback Method |
| dvisc | 0.0005287 | Pa×s | 410.05 | Joback Method |
| dvisc | 0.0008036 | Pa×s | 372.92 | Joback Method |
| dvisc | 0.0013400 | Pa×s | 335.79 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 383.20 | K | 0.70 | NIST Webbook |

# Sources

**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=C10259220&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

# 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

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