# Ethyl-2-chlorobenzoate

**Other names:** Ethyl O-chlorobenzoate
Benzoic acid, 2-chloro-, ethyl ester
2-Chlorobenzoic acid, ethyl ester
**Inchi:** InChI=1S/C9H9ClO2/c1-2-12-9(11)7-5-3-4-6-8(7)10/h3-6H,2H2,1H3
**InchiKey:** RETLCWPMLJPOTP-UHFFFAOYSA-N
**Formula:** C9H9ClO2
**SMILES:** CCOC(=O)c1ccccc1Cl
**Mol. weight [g/mol]:** 184.62
**CAS:** 7335-25-3

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -118.17 | kJ/mol | Joback Method |
| hf | -264.57 | kJ/mol | Joback Method |
| hfus | 19.70 | kJ/mol | Joback Method |
| hvap | 52.11 | kJ/mol | Joback Method |
| log10ws | -2.82 | | Crippen Method |
| logp | 2.517 | | Crippen Method |
| mcvol | 133.590 | ml/mol | McGowan Method |
| pc | 3239.34 | kPa | Joback Method |
| rinpol | 1341.00 | | NIST Webbook |
| rinpol | 1320.00 | | NIST Webbook |
| rinpol | 1342.00 | | NIST Webbook |
| rinpol | 1334.00 | | NIST Webbook |
| rinpol | 1321.00 | | NIST Webbook |
| rinpol | 1327.00 | | NIST Webbook |
| rinpol | 1311.00 | | NIST Webbook |
| rinpol | 1321.00 | | NIST Webbook |
| rinpol | 1309.00 | | NIST Webbook |
| rinpol | 1317.00 | | NIST Webbook |
| rinpol | 1343.10 | | NIST Webbook |
| rinpol | 1322.00 | | NIST Webbook |
| rinpol | 1325.00 | | NIST Webbook |
| rinpol | 1343.10 | | NIST Webbook |
| ripol | 1971.00 | | NIST Webbook |
| ripol | 1964.00 | | NIST Webbook |
| ripol | 1952.00 | | NIST Webbook |

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|---|---|---|---|
| ripol | 1929.00 | | NIST Webbook |
| ripol | 1964.00 | | NIST Webbook |
| ripol | 2007.00 | | NIST Webbook |
| ripol | 1971.00 | | NIST Webbook |
| tb | 516.20 | K | NIST Webbook |
| tc | 772.80 | K | Joback Method |
| tf | 332.21 | K | Joback Method |
| vc | 0.504 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 280.82 | J/mol×K | 550.70 | Joback Method |
| cpg | 292.35 | J/mol×K | 587.72 | Joback Method |
| cpg | 303.20 | J/mol×K | 624.73 | Joback Method |
| cpg | 313.39 | J/mol×K | 661.75 | Joback Method |
| cpg | 322.92 | J/mol×K | 698.76 | Joback Method |
| cpg | 331.82 | J/mol×K | 735.78 | Joback Method |
| cpg | 340.09 | J/mol×K | 772.80 | Joback Method |
| dvisc | 0.0016956 | Pa×s | 332.21 | Joback Method |
| dvisc | 0.0010290 | Pa×s | 368.63 | Joback Method |
| dvisc | 0.0006831 | Pa×s | 405.04 | Joback Method |
| dvisc | 0.0004852 | Pa×s | 441.46 | Joback Method |
| dvisc | 0.0003631 | Pa×s | 477.87 | Joback Method |
| dvisc | 0.0002831 | Pa×s | 514.29 | Joback Method |
| dvisc | 0.0002281 | Pa×s | 550.70 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 396.70 | K | 2.00 | NIST Webbook |

# Sources

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

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|---|---|
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **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=C7335253&Units=SI |

# 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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |