# 4-Ethylbenzoic acid, ethyl ester

**Inchi:** InChI=1S/C11H14O2/c1-3-9-5-7-10(8-6-9)11(12)13-4-2/h5-8H,3-4H2,1-2H3
**InchiKey:** ZPUKPAPWEWUPTC-UHFFFAOYSA-N
**Formula:** C11H14O2
**SMILES:** CCOC(=O)c1ccc(CC)cc1
**Mol. weight [g/mol]:** 178.23
**CAS:** 36207-13-3

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -89.40 | kJ/mol | Joback Method |
| hf | -290.11 | kJ/mol | Joback Method |
| hfus | 20.69 | kJ/mol | Joback Method |
| hvap | 52.17 | kJ/mol | Joback Method |
| log10ws | -2.94 | | Crippen Method |
| logp | 2.426 | | Crippen Method |
| mcvol | 149.530 | ml/mol | McGowan Method |
| pc | 2735.42 | kPa | Joback Method |
| rinpol | 1393.00 | | NIST Webbook |
| rinpol | 1393.00 | | NIST Webbook |
| tb | 559.03 | K | Joback Method |
| tc | 769.35 | K | Joback Method |
| tf | 324.83 | K | Joback Method |
| vc | 0.568 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 346.15 | J/mol×K | 559.03 | Joback Method |
| cpg | 360.31 | J/mol×K | 594.08 | Joback Method |
| cpg | 373.70 | J/mol×K | 629.14 | Joback Method |
| cpg | 386.36 | J/mol×K | 664.19 | Joback Method |
| cpg | 398.29 | J/mol×K | 699.24 | Joback Method |
| cpg | 409.50 | J/mol×K | 734.30 | Joback Method |
| cpg | 420.01 | J/mol×K | 769.35 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0017437 | Pa×s | 324.83 | Joback Method |
| dvisc | 0.0009957 | Pa×s | 363.86 | Joback Method |
| dvisc | 0.0006338 | Pa×s | 402.90 | Joback Method |
| dvisc | 0.0004369 | Pa×s | 441.93 | Joback Method |
| dvisc | 0.0003200 | Pa×s | 480.96 | Joback Method |
| dvisc | 0.0002455 | Pa×s | 520.00 | Joback Method |
| dvisc | 0.0001955 | Pa×s | 559.03 | Joback Method |

# Sources

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|---|---|
| **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=C36207133&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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