# Benzeneacetic acid, «alpha»-hydroxy-«alpha»-phenyl-, ethyl ester

**Other names:** Ethyl benzillate
Ethyl diphenylglycolate

**Inchi:** InChI=1S/C16H16O3/c1-2-19-15(17)16(18,13-9-5-3-6-10-13)14-11-7-4-8-12-14/h3-12,18

**InchiKey:** AIPVNQQMYPWQSX-UHFFFAOYSA-N

**Formula:** C16H16O3

**SMILES:** CCOC(=O)C(O)(c1ccccc1)c1ccccc1

**Mol. weight [g/mol]:** 256.30

**CAS:** 52182-15-7

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -59.24 | kJ/mol | Joback Method |
| hf | -306.29 | kJ/mol | Joback Method |
| hfus | 24.74 | kJ/mol | Joback Method |
| hvap | 80.30 | kJ/mol | Joback Method |
| log10ws | -3.12 | | Crippen Method |
| logp | 2.486 | | Crippen Method |
| mcvol | 202.090 | ml/mol | McGowan Method |
| pc | 2670.78 | kPa | Joback Method |
| tb | 784.08 | K | Joback Method |
| tc | 1011.10 | K | Joback Method |
| tf | 307.00 | K | NIST Webbook |
| vc | 0.748 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 575.23 | J/mol×K | 784.08 | Joback Method |
| cpg | 588.03 | J/mol×K | 821.92 | Joback Method |
| cpg | 599.77 | J/mol×K | 859.75 | Joback Method |
| cpg | 610.53 | J/mol×K | 897.59 | Joback Method |
| cpg | 620.40 | J/mol×K | 935.42 | Joback Method |
| cpg | 629.45 | J/mol×K | 973.26 | Joback Method |
| cpg | 637.76 | J/mol×K | 1011.10 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0008545 | Pa×s | 458.32 | Joback Method |
| dvisc | 0.0003228 | Pa×s | 512.61 | Joback Method |
| dvisc | 0.0001470 | Pa×s | 566.91 | Joback Method |
| dvisc | 0.0000768 | Pa×s | 621.20 | Joback Method |
| dvisc | 0.0000445 | Pa×s | 675.49 | Joback Method |
| dvisc | 0.0000280 | Pa×s | 729.79 | Joback Method |
| dvisc | 0.0000188 | Pa×s | 784.08 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 474.20 | K | 2.80 | NIST Webbook |
| tbrp | 474.00 | K | 2.80 | NIST Webbook |

# Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**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=C52182157&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
**tb:** Normal Boiling Point Temperature

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