# Benzeneacetic acid, 2-phenylethyl ester

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|---|---|
| **Other names:** | Acetic acid, phenyl-, phenethyl ester |
| | «beta»-Phenylethyl phenylacetate |
| | Benzylcarbinyl «alpha»-toluate |
| | Phenylacetic acid, phenethyl ester |
| | Phenylethyl phenylacetate |
| | 2-Phenylethyl phenylacetate |
| | Phenethyl phenylacetate |
| | Phenethyl «alpha»-toluate |
| | 2-Phenylethyl «alpha»-toluate |
| | Phenylacetic acid, 2-phenylethyl ester |
| | NSC 6676 |
| **Inchi:** | InChI=1S/C16H16O2/c17-16(13-15-9-5-2-6-10-15)18-12-11-14-7-3-1-4-8-14/h1-10H,11-1 |
| **InchiKey:** | ZOZIRNMDEZKZHM-UHFFFAOYSA-N |
| **Formula:** | C16H16O2 |
| **SMILES:** | O=C(Cc1ccccc1)OCCc1ccccc1 |
| **Mol. weight [g/mol]:** | 240.30 |
| **CAS:** | 102-20-5 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 74.74 | kJ/mol | Joback Method |
| hf | -145.31 | kJ/mol | Joback Method |
| hfus | 28.07 | kJ/mol | Joback Method |
| hvap | 64.92 | kJ/mol | Joback Method |
| log10ws | -3.59 | | Crippen Method |
| logp | 3.015 | | Crippen Method |
| mcvol | 196.220 | ml/mol | McGowan Method |
| pc | 2388.85 | kPa | Joback Method |
| rinpol | 1919.00 | | NIST Webbook |
| rinpol | 1919.00 | | NIST Webbook |
| rinpol | 1898.00 | | NIST Webbook |
| rinpol | 1898.00 | | NIST Webbook |
| rinpol | 1882.50 | | NIST Webbook |
| rinpol | 1898.00 | | NIST Webbook |
| rinpol | 1924.30 | | NIST Webbook |
| rinpol | 1924.30 | | NIST Webbook |
| ripol | 2618.00 | | NIST Webbook |

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|---|---|---|---|
| ripol | 2618.00 | | NIST Webbook |
| tb | 695.13 | K | Joback Method |
| tc | 928.08 | K | Joback Method |
| tf | 395.08 | K | Joback Method |
| vc | 0.740 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 518.86 | J/mol×K | 695.13 | Joback Method |
| cpg | 587.75 | J/mol×K | 889.25 | Joback Method |
| cpg | 576.23 | J/mol×K | 850.43 | Joback Method |
| cpg | 563.64 | J/mol×K | 811.60 | Joback Method |
| cpg | 549.92 | J/mol×K | 772.78 | Joback Method |
| cpg | 535.01 | J/mol×K | 733.95 | Joback Method |
| cpg | 598.26 | J/mol×K | 928.08 | Joback Method |
| dvisc | 0.0001223 | Pa×s | 695.13 | Joback Method |
| dvisc | 0.0001572 | Pa×s | 645.12 | Joback Method |
| dvisc | 0.0002108 | Pa×s | 595.11 | Joback Method |
| dvisc | 0.0002983 | Pa×s | 545.11 | Joback Method |
| dvisc | 0.0004527 | Pa×s | 495.10 | Joback Method |
| dvisc | 0.0007547 | Pa×s | 445.09 | Joback Method |
| dvisc | 0.0014320 | Pa×s | 395.08 | Joback Method |

# 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=C102205&Units=SI

# Legend

**cpg:** Ideal gas heat capacity
**dvisc:** Dynamic viscosity

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