# Benzenepropanoic acid, 3-phenylpropyl ester

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|---|---|
| **Other names:** | 3-Phenylpropionic acid, 3-phenylpropyl ester |
| | 3-Phenylpropyl 3-phenylpropanoate |
| | 3-phenylpropyl 3-phenylpropionate |
| **Inchi:** | InChI=1S/C18H20O2/c19-18(14-13-17-10-5-2-6-11-17)20-15-7-12-16-8-3-1-4-9-16/h1-6, |
| **InchiKey:** | KLDUFQGXXVNTDL-UHFFFAOYSA-N |
| **Formula:** | C18H20O2 |
| **SMILES:** | O=C(CCc1ccccc1)OCCCc1ccccc1 |
| **Mol. weight [g/mol]:** | 268.35 |
| **CAS:** | 60045-27-4 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 91.58 | kJ/mol | Joback Method |
| hf | -186.59 | kJ/mol | Joback Method |
| hfus | 33.24 | kJ/mol | Joback Method |
| hvap | 69.37 | kJ/mol | Joback Method |
| log10ws | -4.43 | | Crippen Method |
| logp | 3.795 | | Crippen Method |
| mcvol | 224.400 | ml/mol | McGowan Method |
| pc | 1996.55 | kPa | Joback Method |
| rinpol | 2090.00 | | NIST Webbook |
| rinpol | 2115.00 | | NIST Webbook |
| rinpol | 2175.20 | | NIST Webbook |
| rinpol | 2090.00 | | NIST Webbook |
| rinpol | 2175.20 | | NIST Webbook |
| ripol | 2925.00 | | NIST Webbook |
| ripol | 2925.00 | | NIST Webbook |
| tb | 740.89 | K | Joback Method |
| tc | 965.64 | K | Joback Method |
| tf | 417.62 | K | Joback Method |
| vc | 0.852 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 626.67 | J/mol×K | 740.89 | Joback Method |
| cpg | 643.33 | J/mol×K | 778.35 | Joback Method |
| cpg | 658.75 | J/mol×K | 815.81 | Joback Method |
| cpg | 672.98 | J/mol×K | 853.26 | Joback Method |
| cpg | 686.08 | J/mol×K | 890.72 | Joback Method |
| cpg | 698.12 | J/mol×K | 928.18 | Joback Method |
| cpg | 709.15 | J/mol×K | 965.64 | Joback Method |
| dvisc | 0.0012396 | Pa×s | 417.62 | Joback Method |
| dvisc | 0.0006357 | Pa×s | 471.50 | Joback Method |
| dvisc | 0.0003739 | Pa×s | 525.38 | Joback Method |
| dvisc | 0.0002427 | Pa×s | 579.25 | Joback Method |
| dvisc | 0.0001696 | Pa×s | 633.13 | Joback Method |
| dvisc | 0.0001253 | Pa×s | 687.01 | Joback Method |
| dvisc | 0.0000968 | Pa×s | 740.89 | 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=C60045274&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

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