# Ethyl 2-phenoxybutyrate

**Inchi:** InChI=1S/C12H16O3/c1-3-11(12(13)14-4-2)15-10-8-6-5-7-9-10/h5-9,11H,3-4H2,1-2H3
**InchiKey:** IHASFDBVENKSHI-UHFFFAOYSA-N
**Formula:** C12H16O3
**SMILES:** CCOC(=O)C(CC)Oc1ccccc1
**Mol. weight [g/mol]:** 208.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -178.79 | kJ/mol | Joback Method |
| hf | -436.78 | kJ/mol | Joback Method |
| hfus | 21.33 | kJ/mol | Joback Method |
| hvap | 55.76 | kJ/mol | Joback Method |
| log10ws | -2.66 | | Crippen Method |
| logp | 2.407 | | Crippen Method |
| mcvol | 169.490 | ml/mol | McGowan Method |
| pc | 2495.01 | kPa | Joback Method |
| rinpol | 1392.00 | | NIST Webbook |
| rinpol | 1392.00 | | NIST Webbook |
| tb | 598.91 | K | Joback Method |
| tc | 806.97 | K | Joback Method |
| tf | 330.81 | K | Joback Method |
| vc | 0.635 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 420.15 | J/mol×K | 598.91 | Joback Method |
| cpg | 435.37 | J/mol×K | 633.59 | Joback Method |
| cpg | 449.74 | J/mol×K | 668.26 | Joback Method |
| cpg | 463.27 | J/mol×K | 702.94 | Joback Method |
| cpg | 475.99 | J/mol×K | 737.62 | Joback Method |
| cpg | 487.88 | J/mol×K | 772.30 | Joback Method |
| cpg | 498.98 | J/mol×K | 806.97 | Joback Method |
| dvisc | 0.0020694 | Pa×s | 330.81 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0010071 | Pa×s | 375.49 | Joback Method |
| dvisc | 0.0005713 | Pa×s | 420.18 | Joback Method |
| dvisc | 0.0003614 | Pa×s | 464.86 | Joback Method |
| dvisc | 0.0002477 | Pa×s | 509.54 | Joback Method |
| dvisc | 0.0001805 | Pa×s | 554.23 | Joback Method |
| dvisc | 0.0001378 | Pa×s | 598.91 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R543038&Units=SI |
| **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 |

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

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