# Butyric acid, 2-phenyl-, 2-ethylhexyl ester

**Inchi:** InChI=1S/C18H28O2/c1-4-7-11-15(5-2)14-20-18(19)17(6-3)16-12-9-8-10-13-16/h8-10,12
**InchiKey:** PSYOOKKRCIYPNY-UHFFFAOYSA-N
**Formula:** C18H28O2
**SMILES:** CCCCC(CC)COC(=O)C(CC)c1ccccc1
**Mol. weight [g/mol]:** 276.41

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -25.71 | kJ/mol | Joback Method |
| hf | -433.68 | kJ/mol | Joback Method |
| hfus | 32.16 | kJ/mol | Joback Method |
| hvap | 66.32 | kJ/mol | Joback Method |
| log10ws | -5.04 | | Crippen Method |
| logp | 4.940 | | Crippen Method |
| mcvol | 248.160 | ml/mol | McGowan Method |
| pc | 1534.26 | kPa | Joback Method |
| rinpol | 1840.00 | | NIST Webbook |
| rinpol | 1840.00 | | NIST Webbook |
| tb | 713.33 | K | Joback Method |
| tc | 911.04 | K | Joback Method |
| tf | 361.20 | K | Joback Method |
| vc | 0.948 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 711.87 | J/mol×K | 713.33 | Joback Method |
| cpg | 793.20 | J/mol×K | 878.09 | Joback Method |
| cpg | 778.95 | J/mol×K | 845.13 | Joback Method |
| cpg | 763.73 | J/mol×K | 812.18 | Joback Method |
| cpg | 747.50 | J/mol×K | 779.23 | Joback Method |
| cpg | 730.22 | J/mol×K | 746.28 | Joback Method |
| cpg | 806.51 | J/mol×K | 911.04 | Joback Method |
| dvisc | 0.0000818 | Pa×s | 713.33 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001118 | Pa×s | 654.64 | Joback Method |
| dvisc | 0.0001624 | Pa×s | 595.95 | Joback Method |
| dvisc | 0.0002560 | Pa×s | 537.27 | Joback Method |
| dvisc | 0.0004513 | Pa×s | 478.58 | Joback Method |
| dvisc | 0.0009318 | Pa×s | 419.89 | Joback Method |
| dvisc | 0.0024352 | Pa×s | 361.20 | 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=U406860&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 |