# 3-Phenylpropionic acid, 2-methylpentyl ester

**Inchi:** InChI=1S/C15H22O2/c1-3-7-13(2)12-17-15(16)11-10-14-8-5-4-6-9-14/h4-6,8-9,13H,3,7,1
**InchiKey:** DMLLNUIUGYQCJQ-UHFFFAOYSA-N
**Formula:** C15H22O2
**SMILES:** CCCC(C)COC(=O)CCc1ccccc1
**Mol. weight [g/mol]:** 234.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -48.53 | kJ/mol | Joback Method |
| hf | -366.48 | kJ/mol | Joback Method |
| hfus | 27.91 | kJ/mol | Joback Method |
| hvap | 60.03 | kJ/mol | Joback Method |
| log10ws | -3.83 | | Crippen Method |
| logp | 3.599 | | Crippen Method |
| mcvol | 205.890 | ml/mol | McGowan Method |
| pc | 1935.54 | kPa | Joback Method |
| rinpol | 1745.00 | | NIST Webbook |
| rinpol | 1745.00 | | NIST Webbook |
| tb | 645.13 | K | Joback Method |
| tc | 846.21 | K | Joback Method |
| tf | 342.39 | K | Joback Method |
| vc | 0.785 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 546.83 | J/mol×K | 645.13 | Joback Method |
| cpg | 563.95 | J/mol×K | 678.64 | Joback Method |
| cpg | 580.10 | J/mol×K | 712.16 | Joback Method |
| cpg | 595.30 | J/mol×K | 745.67 | Joback Method |
| cpg | 609.57 | J/mol×K | 779.18 | Joback Method |
| cpg | 622.96 | J/mol×K | 812.70 | Joback Method |
| cpg | 635.49 | J/mol×K | 846.21 | Joback Method |
| dvisc | 0.0024547 | Pa×s | 342.39 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0010907 | Pa×s | 392.85 | Joback Method |
| dvisc | 0.0005830 | Pa×s | 443.30 | Joback Method |
| dvisc | 0.0003541 | Pa×s | 493.76 | Joback Method |
| dvisc | 0.0002360 | Pa×s | 544.22 | Joback Method |
| dvisc | 0.0001684 | Pa×s | 594.67 | Joback Method |
| dvisc | 0.0001267 | Pa×s | 645.13 | Joback Method |

# Sources

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|---|---|
| **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=U354738&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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