# Hexyl 2-phenoxypropionate

**Inchi:** InChI=1S/C15H22O3/c1-3-4-5-9-12-17-15(16)13(2)18-14-10-7-6-8-11-14/h6-8,10-11,13H
**InchiKey:** KSVPNNZOLYKFND-UHFFFAOYSA-N
**Formula:** C15H22O3
**SMILES:** CCCCCCOC(=O)C(C)Oc1ccccc1
**Mol. weight [g/mol]:** 250.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -153.53 | kJ/mol | Joback Method |
| hf | -498.70 | kJ/mol | Joback Method |
| hfus | 29.10 | kJ/mol | Joback Method |
| hvap | 62.44 | kJ/mol | Joback Method |
| log10ws | -3.91 | | Crippen Method |
| logp | 3.577 | | Crippen Method |
| mcvol | 211.760 | ml/mol | McGowan Method |
| pc | 1906.90 | kPa | Joback Method |
| rinpol | 1684.00 | | NIST Webbook |
| tb | 667.55 | K | Joback Method |
| tc | 867.02 | K | Joback Method |
| tf | 364.62 | K | Joback Method |
| vc | 0.803 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 574.87 | J/mol×K | 667.55 | Joback Method |
| cpg | 591.60 | J/mol×K | 700.80 | Joback Method |
| cpg | 607.37 | J/mol×K | 734.04 | Joback Method |
| cpg | 622.21 | J/mol×K | 767.29 | Joback Method |
| cpg | 636.13 | J/mol×K | 800.53 | Joback Method |
| cpg | 649.15 | J/mol×K | 833.78 | Joback Method |
| cpg | 661.27 | J/mol×K | 867.02 | Joback Method |
| dvisc | 0.0016953 | Pa×s | 364.62 | Joback Method |
| dvisc | 0.0007912 | Pa×s | 415.11 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0004356 | Pa×s | 465.60 | Joback Method |
| dvisc | 0.0002696 | Pa×s | 516.09 | Joback Method |
| dvisc | 0.0001817 | Pa×s | 566.57 | Joback Method |
| dvisc | 0.0001306 | Pa×s | 617.06 | Joback Method |
| dvisc | 0.0000987 | Pa×s | 667.55 | Joback Method |

# Sources

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|---|---|
| **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=R543216&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |