# 2-Phenoxyethyl undecanoate

**Inchi:** InChI=1S/C19H30O3/c1-2-3-4-5-6-7-8-12-15-19(20)22-17-16-21-18-13-10-9-11-14-18/h9
**InchiKey:** YHLMXXACBOHIQC-UHFFFAOYSA-N
**Formula:** C19H30O3
**SMILES:** CCCCCCCCCCC(=O)OCCOc1ccccc1
**Mol. weight [g/mol]:** 306.44

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -117.41 | kJ/mol | Joback Method |
| hf | -575.98 | kJ/mol | Joback Method |
| hfus | 42.98 | kJ/mol | Joback Method |
| hvap | 71.73 | kJ/mol | Joback Method |
| log10ws | -5.48 | | Crippen Method |
| logp | 5.139 | | Crippen Method |
| mcvol | 268.120 | ml/mol | McGowan Method |
| pc | 1390.22 | kPa | Joback Method |
| rinpol | 2221.00 | | NIST Webbook |
| tb | 759.51 | K | Joback Method |
| tc | 950.63 | K | Joback Method |
| tf | 424.70 | K | Joback Method |
| vc | 1.034 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 798.38 | J/mol×K | 759.51 | Joback Method |
| cpg | 816.03 | J/mol×K | 791.36 | Joback Method |
| cpg | 832.64 | J/mol×K | 823.22 | Joback Method |
| cpg | 848.24 | J/mol×K | 855.07 | Joback Method |
| cpg | 862.84 | J/mol×K | 886.92 | Joback Method |
| cpg | 876.48 | J/mol×K | 918.77 | Joback Method |
| cpg | 889.18 | J/mol×K | 950.63 | Joback Method |
| dvisc | 0.0009798 | Pa×s | 424.70 | Joback Method |
| dvisc | 0.0004782 | Pa×s | 480.50 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0002710 | Pa×s | 536.30 | Joback Method |
| dvisc | 0.0001709 | Pa×s | 592.11 | Joback Method |
| dvisc | 0.0001167 | Pa×s | 647.91 | Joback Method |
| dvisc | 0.0000846 | Pa×s | 703.71 | Joback Method |
| dvisc | 0.0000644 | Pa×s | 759.51 | 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=R540891&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 |