# 2-Phenoxyethyl pentadecanoate

**Inchi:** InChI=1S/C23H38O3/c1-2-3-4-5-6-7-8-9-10-11-12-16-19-23(24)26-21-20-25-22-17-14-13
**InchiKey:** JBDLVZUAMGDPCD-UHFFFAOYSA-N
**Formula:** C23H38O3
**SMILES:** CCCCCCCCCCCCCCC(=O)OCCOc1ccccc1
**Mol. weight [g/mol]:** 362.55

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -83.73 | kJ/mol | Joback Method |
| hf | -658.54 | kJ/mol | Joback Method |
| hfus | 53.34 | kJ/mol | Joback Method |
| hvap | 80.63 | kJ/mol | Joback Method |
| log10ws | -7.15 | | Crippen Method |
| logp | 6.700 | | Crippen Method |
| mcvol | 324.480 | ml/mol | McGowan Method |
| pc | 1063.79 | kPa | Joback Method |
| rinpol | 2650.00 | | NIST Webbook |
| tb | 851.03 | K | Joback Method |
| tc | 1046.21 | K | Joback Method |
| tf | 469.78 | K | Joback Method |
| vc | 1.258 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1037.81 | J/mol×K | 851.03 | Joback Method |
| cpg | 1056.42 | J/mol×K | 883.56 | Joback Method |
| cpg | 1073.83 | J/mol×K | 916.09 | Joback Method |
| cpg | 1090.07 | J/mol×K | 948.62 | Joback Method |
| cpg | 1105.17 | J/mol×K | 981.15 | Joback Method |
| cpg | 1119.17 | J/mol×K | 1013.68 | Joback Method |
| cpg | 1132.11 | J/mol×K | 1046.21 | Joback Method |
| dvisc | 0.0006445 | Pa×s | 469.78 | Joback Method |
| dvisc | 0.0003012 | Pa×s | 533.32 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0001655 | Pa×s | 596.86 | Joback Method |
| dvisc | 0.0001020 | Pa×s | 660.40 | Joback Method |
| dvisc | 0.0000685 | Pa×s | 723.95 | Joback Method |
| dvisc | 0.0000490 | Pa×s | 787.49 | Joback Method |
| dvisc | 0.0000369 | Pa×s | 851.03 | Joback Method |

# Sources

**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=R540866&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