# Terephthalic acid, heptyl 2-phenoxyethyl ester

**Inchi:** InChI=1S/C23H28O5/c1-2-3-4-5-9-16-27-22(24)19-12-14-20(15-13-19)23(25)28-18-17-2
**InchiKey:** QSTIQWBMWNWQLP-UHFFFAOYSA-N
**Formula:** C23H28O5
**SMILES:** CCCCCCCOC(=O)c1ccc(C(=O)OCCOc2ccccc2)cc1
**Mol. weight [g/mol]:** 384.47

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -214.87 | kJ/mol | Joback Method |
| hf | -678.28 | kJ/mol | Joback Method |
| hfus | 49.78 | kJ/mol | Joback Method |
| hvap | 92.73 | kJ/mol | Joback Method |
| log10ws | -6.24 | | Crippen Method |
| logp | 5.050 | | Crippen Method |
| mcvol | 308.160 | ml/mol | McGowan Method |
| pc | 1367.69 | kPa | Joback Method |
| rinpol | 3160.00 | | NIST Webbook |
| rinpol | 3160.00 | | NIST Webbook |
| tb | 958.98 | K | Joback Method |
| tc | 1182.01 | K | Joback Method |
| tf | 580.88 | K | Joback Method |
| vc | 1.173 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 984.53 | J/mol×K | 958.98 | Joback Method |
| cpg | 998.05 | J/mol×K | 996.15 | Joback Method |
| cpg | 1010.09 | J/mol×K | 1033.32 | Joback Method |
| cpg | 1020.69 | J/mol×K | 1070.49 | Joback Method |
| cpg | 1029.87 | J/mol×K | 1107.66 | Joback Method |
| cpg | 1037.67 | J/mol×K | 1144.84 | Joback Method |
| cpg | 1044.12 | J/mol×K | 1182.01 | Joback Method |
| dvisc | 0.0002656 | Pa×s | 580.88 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001511 | Pa×s | 643.90 | Joback Method |
| dvisc | 0.0000950 | Pa×s | 706.91 | Joback Method |
| dvisc | 0.0000644 | Pa×s | 769.93 | Joback Method |
| dvisc | 0.0000464 | Pa×s | 832.95 | Joback Method |
| dvisc | 0.0000349 | Pa×s | 895.96 | Joback Method |
| dvisc | 0.0000273 | Pa×s | 958.98 | 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=U416046&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

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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 |