# Phthalic acid, 6-methylhept-2-yl undecyl ester

**Inchi:** InChI=1S/C27H44O4/c1-5-6-7-8-9-10-11-12-15-21-30-26(28)24-19-13-14-20-25(24)27(2
**InchiKey:** UUYHGTCDUTZBSR-UHFFFAOYSA-N
**Formula:** C27H44O4
**SMILES:** CCCCCCCCCCCOC(=O)c1ccccc1C(=O)OC(C)CCCC(C)C
**Mol. weight [g/mol]:** 432.64

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -193.48 | kJ/mol | Joback Method |
| hf | -875.71 | kJ/mol | Joback Method |
| hfus | 57.87 | kJ/mol | Joback Method |
| hvap | 96.17 | kJ/mol | Joback Method |
| log10ws | -8.94 | | Crippen Method |
| logp | 7.746 | | Crippen Method |
| mcvol | 382.410 | ml/mol | McGowan Method |
| pc | 872.22 | kPa | Joback Method |
| rinpol | 2910.00 | | NIST Webbook |
| tb | 1000.52 | K | Joback Method |
| tc | 1225.74 | K | Joback Method |
| tf | 547.31 | K | Joback Method |
| vc | 1.476 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1307.09 | J/mol×K | 1000.52 | Joback Method |
| cpg | 1379.34 | J/mol×K | 1188.20 | Joback Method |
| cpg | 1367.98 | J/mol×K | 1150.67 | Joback Method |
| cpg | 1355.13 | J/mol×K | 1113.13 | Joback Method |
| cpg | 1340.74 | J/mol×K | 1075.59 | Joback Method |
| cpg | 1324.74 | J/mol×K | 1038.06 | Joback Method |
| cpg | 1389.27 | J/mol×K | 1225.74 | Joback Method |
| dvisc | 0.0000162 | Pa×s | 1000.52 | Joback Method |
| dvisc | 0.0000218 | Pa×s | 924.99 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000309 | Pa×s | 849.45 | Joback Method |
| dvisc | 0.0000470 | Pa×s | 773.91 | Joback Method |
| dvisc | 0.0000783 | Pa×s | 698.38 | Joback Method |
| dvisc | 0.0001475 | Pa×s | 622.84 | Joback Method |
| dvisc | 0.0003310 | Pa×s | 547.31 | 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=U377965&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 |