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

**Inchi:** InChI=1S/C29H48O4/c1-5-6-7-8-9-10-11-12-13-14-17-23-32-28(30)26-21-15-16-22-27(2
**InchiKey:** ILTIGDBNVUDGGH-UHFFFAOYSA-N
**Formula:** C29H48O4
**SMILES:** CCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OC(C)CCCC(C)C
**Mol. weight [g/mol]:** 460.69

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -176.64 | kJ/mol | Joback Method |
| hf | -916.99 | kJ/mol | Joback Method |
| hfus | 63.05 | kJ/mol | Joback Method |
| hvap | 100.62 | kJ/mol | Joback Method |
| log10ws | -9.78 | | Crippen Method |
| logp | 8.526 | | Crippen Method |
| mcvol | 410.590 | ml/mol | McGowan Method |
| pc | 781.12 | kPa | Joback Method |
| rinpol | 3105.00 | | NIST Webbook |
| rinpol | 3105.00 | | NIST Webbook |
| tb | 1046.28 | K | Joback Method |
| tc | 1286.84 | K | Joback Method |
| tf | 569.85 | K | Joback Method |
| vc | 1.587 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1433.52 | J/mol×K | 1046.28 | Joback Method |
| cpg | 1451.74 | J/mol×K | 1086.37 | Joback Method |
| cpg | 1468.04 | J/mol×K | 1126.47 | Joback Method |
| cpg | 1482.52 | J/mol×K | 1166.56 | Joback Method |
| cpg | 1495.24 | J/mol×K | 1206.65 | Joback Method |
| cpg | 1506.29 | J/mol×K | 1246.75 | Joback Method |
| cpg | 1515.75 | J/mol×K | 1286.84 | Joback Method |
| dvisc | 0.0002531 | Pa×s | 569.85 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001111 | Pa×s | 649.25 | Joback Method |
| dvisc | 0.0000584 | Pa×s | 728.66 | Joback Method |
| dvisc | 0.0000348 | Pa×s | 808.06 | Joback Method |
| dvisc | 0.0000228 | Pa×s | 887.47 | Joback Method |
| dvisc | 0.0000160 | Pa×s | 966.88 | Joback Method |
| dvisc | 0.0000118 | Pa×s | 1046.28 | Joback Method |

# Sources

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|---|---|
| **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=U377967&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 |