# Phthalic acid, 3,3-dimethylbut-2-yl pentadecyl ester

**Inchi:** InChI=1S/C29H48O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-20-23-32-27(30)25-21-18-19-

**InchiKey:** OYBUWNFSYRLNAS-UHFFFAOYSA-N

**Formula:** C29H48O4

**SMILES:** CCCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OC(C)C(C)(C)C

**Mol. weight [g/mol]:** 460.69

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -171.36 | kJ/mol | Joback Method |
| hf | -920.46 | kJ/mol | Joback Method |
| hfus | 59.15 | kJ/mol | Joback Method |
| hvap | 99.71 | kJ/mol | Joback Method |
| log10ws | -9.78 | | Crippen Method |
| logp | 8.526 | | Crippen Method |
| mcvol | 410.590 | ml/mol | McGowan Method |
| pc | 785.95 | kPa | Joback Method |
| rinpol | 3137.00 | | NIST Webbook |
| tb | 1043.49 | K | Joback Method |
| tc | 1280.94 | K | Joback Method |
| tf | 587.27 | K | Joback Method |
| vc | 1.583 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1433.20 | J/mol×K | 1043.49 | Joback Method |
| cpg | 1451.61 | J/mol×K | 1083.07 | Joback Method |
| cpg | 1468.35 | J/mol×K | 1122.64 | Joback Method |
| cpg | 1483.54 | J/mol×K | 1162.22 | Joback Method |
| cpg | 1497.27 | J/mol×K | 1201.79 | Joback Method |
| cpg | 1509.66 | J/mol×K | 1241.37 | Joback Method |
| cpg | 1520.81 | J/mol×K | 1280.94 | Joback Method |
| dvisc | 0.0001963 | Pa×s | 587.27 | Joback Method |
| dvisc | 0.0000892 | Pa×s | 663.31 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000477 | Pa×s | 739.34 | Joback Method |
| dvisc | 0.0000287 | Pa×s | 815.38 | Joback Method |
| dvisc | 0.0000188 | Pa×s | 891.42 | Joback Method |
| dvisc | 0.0000132 | Pa×s | 967.45 | Joback Method |
| dvisc | 0.0000097 | Pa×s | 1043.49 | 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=U357014&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 |