# Phthalic acid, heptadecyl 2,4,4-trimethylpentyl ester

**Inchi:** InChI=1S/C33H56O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-25-36-31(34)29-23-

**InchiKey:** BMJSTJWHNVDJKL-UHFFFAOYSA-N

**Formula:** C33H56O4

**SMILES:** CCCCCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCC(C)CC(C)(C)C

**Mol. weight [g/mol]:** 516.80

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -137.68 | kJ/mol | Joback Method |
| hf | -1003.02 | kJ/mol | Joback Method |
| hfus | 69.52 | kJ/mol | Joback Method |
| hvap | 108.62 | kJ/mol | Joback Method |
| log10ws | -11.10 | | Crippen Method |
| logp | 9.944 | | Crippen Method |
| mcvol | 466.950 | ml/mol | McGowan Method |
| pc | 640.60 | kPa | Joback Method |
| rinpol | 3490.00 | | NIST Webbook |
| tb | 1135.01 | K | Joback Method |
| tc | 1415.49 | K | Joback Method |
| tf | 632.35 | K | Joback Method |
| vc | 1.806 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1690.20 | J/mol×K | 1135.01 | Joback Method |
| cpg | 1772.48 | J/mol×K | 1368.74 | Joback Method |
| cpg | 1759.56 | J/mol×K | 1322.00 | Joback Method |
| cpg | 1745.08 | J/mol×K | 1275.25 | Joback Method |
| cpg | 1728.82 | J/mol×K | 1228.50 | Joback Method |
| cpg | 1710.60 | J/mol×K | 1181.76 | Joback Method |
| cpg | 1784.03 | J/mol×K | 1415.49 | Joback Method |
| dvisc | 0.0000050 | Pa×s | 1135.01 | Joback Method |
| dvisc | 0.0000068 | Pa×s | 1051.23 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000098 | Pa×s | 967.46 | Joback Method |
| dvisc | 0.0000152 | Pa×s | 883.68 | Joback Method |
| dvisc | 0.0000256 | Pa×s | 799.90 | Joback Method |
| dvisc | 0.0000488 | Pa×s | 716.13 | Joback Method |
| dvisc | 0.0001104 | Pa×s | 632.35 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U377783&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |