# Phthalic acid, heptadecyl 4-methylhept-3-yl ester

**Inchi:** InChI=1S/C33H56O4/c1-5-8-9-10-11-12-13-14-15-16-17-18-19-20-23-27-36-32(34)29-25

**InchiKey:** XCOMBEJEBSJORI-UHFFFAOYSA-N

**Formula:** C33H56O4

**SMILES:** CCCCCCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OC(CC)C(C)CCC

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

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -142.96 | kJ/mol | Joback Method |
| hf | -999.55 | kJ/mol | Joback Method |
| hfus | 73.41 | kJ/mol | Joback Method |
| hvap | 109.53 | kJ/mol | Joback Method |
| log10ws | -11.45 | | Crippen Method |
| logp | 10.086 | | Crippen Method |
| mcvol | 466.950 | ml/mol | McGowan Method |
| pc | 637.05 | kPa | Joback Method |
| rinpol | 3501.00 | | NIST Webbook |
| rinpol | 3501.00 | | NIST Webbook |
| tb | 1137.80 | K | Joback Method |
| tc | 1425.65 | K | Joback Method |
| tf | 614.93 | K | Joback Method |
| vc | 1.812 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1689.45 | J/mol×K | 1137.80 | Joback Method |
| cpg | 1763.06 | J/mol×K | 1377.68 | Joback Method |
| cpg | 1753.01 | J/mol×K | 1329.70 | Joback Method |
| cpg | 1740.80 | J/mol×K | 1281.73 | Joback Method |
| cpg | 1726.25 | J/mol×K | 1233.75 | Joback Method |
| cpg | 1709.19 | J/mol×K | 1185.78 | Joback Method |
| cpg | 1771.10 | J/mol×K | 1425.65 | Joback Method |
| dvisc | 0.0000062 | Pa×s | 1137.80 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000084 | Pa×s | 1050.65 | Joback Method |
| dvisc | 0.0000121 | Pa×s | 963.51 | Joback Method |
| dvisc | 0.0000187 | Pa×s | 876.37 | Joback Method |
| dvisc | 0.0000318 | Pa×s | 789.22 | Joback Method |
| dvisc | 0.0000617 | Pa×s | 702.08 | Joback Method |
| dvisc | 0.0001443 | Pa×s | 614.93 | Joback Method |

# Sources

| | |
|---|---|
| **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=U377952&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 |