# Pimelic acid, 2-pentyl tetradecyl ester

**Inchi:** InChI=1S/C26H50O4/c1-4-6-7-8-9-10-11-12-13-14-15-19-23-29-25(27)21-17-16-18-22-2
**InchiKey:** PBPRIBXICAMZHY-UHFFFAOYSA-N
**Formula:** C26H50O4
**SMILES:** CCCCCCCCCCCCCCOC(=O)CCCCCC(=O)OC(C)CCC
**Mol. weight [g/mol]:** 426.67

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -302.24 | kJ/mol | Joback Method |
| hf | -1074.85 | kJ/mol | Joback Method |
| hfus | 65.15 | kJ/mol | Joback Method |
| hvap | 91.39 | kJ/mol | Joback Method |
| log10ws | -8.54 | | Crippen Method |
| logp | 7.913 | | Crippen Method |
| mcvol | 392.080 | ml/mol | McGowan Method |
| pc | 765.64 | kPa | Joback Method |
| rinpol | 2877.00 | | NIST Webbook |
| rinpol | 2877.00 | | NIST Webbook |
| tb | 946.42 | K | Joback Method |
| tc | 1164.49 | K | Joback Method |
| tf | 512.10 | K | Joback Method |
| vc | 1.534 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1345.59 | J/mol×K | 946.42 | Joback Method |
| cpg | 1366.80 | J/mol×K | 982.76 | Joback Method |
| cpg | 1386.34 | J/mol×K | 1019.11 | Joback Method |
| cpg | 1404.25 | J/mol×K | 1055.45 | Joback Method |
| cpg | 1420.58 | J/mol×K | 1091.80 | Joback Method |
| cpg | 1435.40 | J/mol×K | 1128.14 | Joback Method |
| cpg | 1448.73 | J/mol×K | 1164.49 | Joback Method |
| dvisc | 0.0004671 | Pa×s | 512.10 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001988 | Pa×s | 584.49 | Joback Method |
| dvisc | 0.0001021 | Pa×s | 656.87 | Joback Method |
| dvisc | 0.0000599 | Pa×s | 729.26 | Joback Method |
| dvisc | 0.0000387 | Pa×s | 801.65 | Joback Method |
| dvisc | 0.0000268 | Pa×s | 874.03 | Joback Method |
| dvisc | 0.0000197 | Pa×s | 946.42 | Joback Method |

# Sources

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|---|---|
| **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=U393800&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |