# Pimelic acid, 3,7-dimethyloctyl tetradecyl ester

**Inchi:** InChI=1S/C31H60O4/c1-5-6-7-8-9-10-11-12-13-14-15-19-26-34-30(32)23-17-16-18-24-3
**InchiKey:** JEUHFJUUSQVIJD-UHFFFAOYSA-N
**Formula:** C31H60O4
**SMILES:** CCCCCCCCCCCCCCOC(=O)CCCCCC(=O)OCCC(C)CCCC(C)C
**Mol. weight [g/mol]:** 496.81

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -262.58 | kJ/mol | Joback Method |
| hf | -1183.33 | kJ/mol | Joback Method |
| hfus | 74.57 | kJ/mol | Joback Method |
| hvap | 102.14 | kJ/mol | Joback Method |
| log10ws | -10.04 | | Crippen Method |
| logp | 9.577 | | Crippen Method |
| mcvol | 462.530 | ml/mol | McGowan Method |
| pc | 598.97 | kPa | Joback Method |
| rinpol | 3356.00 | | NIST Webbook |
| rinpol | 3356.00 | | NIST Webbook |
| tb | 1060.38 | K | Joback Method |
| tc | 1335.48 | K | Joback Method |
| tf | 553.45 | K | Joback Method |
| vc | 1.808 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1671.19 | J/mol×K | 1060.38 | Joback Method |
| cpg | 1695.52 | J/mol×K | 1106.23 | Joback Method |
| cpg | 1717.12 | J/mol×K | 1152.08 | Joback Method |
| cpg | 1736.12 | J/mol×K | 1197.93 | Joback Method |
| cpg | 1752.66 | J/mol×K | 1243.78 | Joback Method |
| cpg | 1766.86 | J/mol×K | 1289.63 | Joback Method |
| cpg | 1778.86 | J/mol×K | 1335.48 | Joback Method |
| dvisc | 0.0002633 | Pa×s | 553.45 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0001001 | Pa×s | 637.94 | Joback Method |
| dvisc | 0.0000477 | Pa×s | 722.43 | Joback Method |
| dvisc | 0.0000266 | Pa×s | 806.91 | Joback Method |
| dvisc | 0.0000165 | Pa×s | 891.40 | Joback Method |
| dvisc | 0.0000112 | Pa×s | 975.89 | Joback Method |
| dvisc | 0.0000080 | Pa×s | 1060.38 | 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=U393747&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 |

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