# Adipic acid, 2,4-dimethylpent-3-yl tetradecyl ester

**Inchi:** InChI=1S/C27H52O4/c1-6-7-8-9-10-11-12-13-14-15-16-19-22-30-25(28)20-17-18-21-26(

**InchiKey:** BFILCLQUIFJKIW-UHFFFAOYSA-N

**Formula:** C27H52O4

**SMILES:** CCCCCCCCCCCCCCOC(=O)CCCCC(=O)OC(C(C)C)C(C)C

**Mol. weight [g/mol]:** 440.70

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -298.70 | kJ/mol | Joback Method |
| hf | -1106.05 | kJ/mol | Joback Method |
| hfus | 60.69 | kJ/mol | Joback Method |
| hvap | 92.84 | kJ/mol | Joback Method |
| log10ws | -8.48 | | Crippen Method |
| logp | 8.015 | | Crippen Method |
| mcvol | 406.170 | ml/mol | McGowan Method |
| pc | 732.84 | kPa | Joback Method |
| rinpol | 2884.00 | | NIST Webbook |
| tb | 968.42 | K | Joback Method |
| tc | 1192.39 | K | Joback Method |
| tf | 493.37 | K | Joback Method |
| vc | 1.577 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1410.70 | J/mol×K | 968.42 | Joback Method |
| cpg | 1432.11 | J/mol×K | 1005.75 | Joback Method |
| cpg | 1451.72 | J/mol×K | 1043.08 | Joback Method |
| cpg | 1469.56 | J/mol×K | 1080.40 | Joback Method |
| cpg | 1485.71 | J/mol×K | 1117.73 | Joback Method |
| cpg | 1500.22 | J/mol×K | 1155.06 | Joback Method |
| cpg | 1513.15 | J/mol×K | 1192.39 | Joback Method |
| dvisc | 0.0005544 | Pa×s | 493.37 | Joback Method |
| dvisc | 0.0001964 | Pa×s | 572.55 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000895 | Pa×s | 651.72 | Joback Method |
| dvisc | 0.0000484 | Pa×s | 730.89 | Joback Method |
| dvisc | 0.0000295 | Pa×s | 810.07 | Joback Method |
| dvisc | 0.0000196 | Pa×s | 889.25 | Joback Method |
| dvisc | 0.0000140 | Pa×s | 968.42 | Joback Method |

# Sources

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|---|---|
| **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=U353531&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 |