# Terephthalic acid, 4-heptyl tetradecyl ester

**Inchi:** InChI=1S/C29H48O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-24-32-28(30)25-20-22-26(23-
**InchiKey:** GUICPMWUZAXWEO-UHFFFAOYSA-N
**Formula:** C29H48O4
**SMILES:** CCCCCCCCCCCCCCCOC(=O)c1ccc(C(=O)OC(CCC)CCC)cc1
**Mol. weight [g/mol]:** 460.69

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -174.20 | kJ/mol | Joback Method |
| hf | -911.71 | kJ/mol | Joback Method |
| hfus | 66.57 | kJ/mol | Joback Method |
| hvap | 101.01 | kJ/mol | Joback Method |
| log10ws | -10.02 | | Crippen Method |
| logp | 8.670 | | Crippen Method |
| mcvol | 410.590 | ml/mol | McGowan Method |
| pc | 777.64 | kPa | Joback Method |
| rinpol | 3262.00 | | NIST Webbook |
| tb | 1046.72 | K | Joback Method |
| tc | 1288.88 | K | Joback Method |
| tf | 584.85 | K | Joback Method |
| vc | 1.593 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1433.30 | J/mol×K | 1046.72 | Joback Method |
| cpg | 1451.71 | J/mol×K | 1087.08 | Joback Method |
| cpg | 1468.21 | J/mol×K | 1127.44 | Joback Method |
| cpg | 1482.86 | J/mol×K | 1167.80 | Joback Method |
| cpg | 1495.77 | J/mol×K | 1208.16 | Joback Method |
| cpg | 1507.00 | J/mol×K | 1248.52 | Joback Method |
| cpg | 1516.63 | J/mol×K | 1288.88 | Joback Method |
| dvisc | 0.0002283 | Pa×s | 584.85 | Joback Method |
| dvisc | 0.0001073 | Pa×s | 661.83 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000590 | Pa×s | 738.81 | Joback Method |
| dvisc | 0.0000363 | Pa×s | 815.78 | Joback Method |
| dvisc | 0.0000243 | Pa×s | 892.76 | Joback Method |
| dvisc | 0.0000173 | Pa×s | 969.74 | Joback Method |
| dvisc | 0.0000130 | Pa×s | 1046.72 | 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=U356164&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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