# Terephthalic acid, heptyl 2,4,4-trimethylpentyl ester

**Inchi:** InChI=1S/C23H36O4/c1-6-7-8-9-10-15-26-21(24)19-11-13-20(14-12-19)22(25)27-17-18(

**InchiKey:** DOLUYRZCYWOENS-UHFFFAOYSA-N

**Formula:** C23H36O4

**SMILES:** CCCCCCCOC(=O)c1ccc(C(=O)OCC(C)CC(C)(C)C)cc1

**Mol. weight [g/mol]:** 376.53

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -221.88 | kJ/mol | Joback Method |
| hf | -796.62 | kJ/mol | Joback Method |
| hfus | 43.62 | kJ/mol | Joback Method |
| hvap | 86.36 | kJ/mol | Joback Method |
| log10ws | -6.91 | | Crippen Method |
| logp | 6.043 | | Crippen Method |
| mcvol | 326.050 | ml/mol | McGowan Method |
| pc | 1117.81 | kPa | Joback Method |
| rinpol | 2770.00 | | NIST Webbook |
| rinpol | 2770.00 | | NIST Webbook |
| tb | 906.21 | K | Joback Method |
| tc | 1115.53 | K | Joback Method |
| tf | 519.65 | K | Joback Method |
| vc | 1.246 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1058.87 | J/mol×K | 906.21 | Joback Method |
| cpg | 1075.76 | J/mol×K | 941.10 | Joback Method |
| cpg | 1091.37 | J/mol×K | 975.98 | Joback Method |
| cpg | 1105.75 | J/mol×K | 1010.87 | Joback Method |
| cpg | 1118.97 | J/mol×K | 1045.76 | Joback Method |
| cpg | 1131.08 | J/mol×K | 1080.64 | Joback Method |
| cpg | 1142.12 | J/mol×K | 1115.53 | Joback Method |
| dvisc | 0.0004367 | Pa×s | 519.65 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002089 | Pa×s | 584.08 | Joback Method |
| dvisc | 0.0001157 | Pa×s | 648.50 | Joback Method |
| dvisc | 0.0000713 | Pa×s | 712.93 | Joback Method |
| dvisc | 0.0000476 | Pa×s | 777.36 | Joback Method |
| dvisc | 0.0000338 | Pa×s | 841.78 | Joback Method |
| dvisc | 0.0000252 | Pa×s | 906.21 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U416013&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# 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 |