# Terephthalic acid, hexyl 5-methylhex-2-yl ester

**Inchi:** InChI=1S/C21H32O4/c1-5-6-7-8-15-24-20(22)18-11-13-19(14-12-18)21(23)25-17(4)10-9
**InchiKey:** WQVQSTKLSBPJIM-UHFFFAOYSA-N
**Formula:** C21H32O4
**SMILES:** CCCCCCOC(=O)c1ccc(C(=O)OC(C)CCC(C)C)cc1
**Mol. weight [g/mol]:** 348.48

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -244.00 | kJ/mol | Joback Method |
| hf | -751.87 | kJ/mol | Joback Method |
| hfus | 42.33 | kJ/mol | Joback Method |
| hvap | 82.81 | kJ/mol | Joback Method |
| log10ws | -6.43 | | Crippen Method |
| logp | 5.405 | | Crippen Method |
| mcvol | 297.870 | ml/mol | McGowan Method |
| pc | 1266.45 | kPa | Joback Method |
| rinpol | 2767.00 | | NIST Webbook |
| rinpol | 2767.00 | | NIST Webbook |
| tb | 863.24 | K | Joback Method |
| tc | 1067.43 | K | Joback Method |
| tf | 479.69 | K | Joback Method |
| vc | 1.139 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 938.15 | J/mol×K | 863.24 | Joback Method |
| cpg | 954.70 | J/mol×K | 897.27 | Joback Method |
| cpg | 970.02 | J/mol×K | 931.30 | Joback Method |
| cpg | 984.13 | J/mol×K | 965.34 | Joback Method |
| cpg | 997.06 | J/mol×K | 999.37 | Joback Method |
| cpg | 1008.83 | J/mol×K | 1033.40 | Joback Method |
| cpg | 1019.48 | J/mol×K | 1067.43 | Joback Method |
| dvisc | 0.0006933 | Pa×s | 479.69 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0003257 | Pa×s | 543.62 | Joback Method |
| dvisc | 0.0001793 | Pa×s | 607.54 | Joback Method |
| dvisc | 0.0001106 | Pa×s | 671.47 | Joback Method |
| dvisc | 0.0000742 | Pa×s | 735.39 | Joback Method |
| dvisc | 0.0000531 | Pa×s | 799.32 | Joback Method |
| dvisc | 0.0000399 | Pa×s | 863.24 | 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=U382999&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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