

Terephthalic acid, 4-methylhept-3-yl pentyl ester

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|----------------------|---|
| Inchi: | InChI=1S/C21H32O4/c1-5-8-9-15-24-20(22)17-11-13-18(14-12-17)21(23)25-19(7-3)16(4) |
| InchiKey: | OQUNCXQOCJVSEU-UHFFFAOYSA-N |
| Formula: | C21H32O4 |
| SMILES: | CCCCCOC(=O)c1ccc(C(=O)OC(CC)C(C)CCC)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 |
| mvol | 297.870 | ml/mol | McGowan Method |
| pc | 1266.45 | kPa | Joback Method |
| rinpol | 2560.00 | | NIST Webbook |
| rinpol | 2560.00 | | NIST Webbook |
| tb | 863.24 | K | Joback Method |
| tc | 1067.43 | K | Joback Method |
| tf | 479.69 | K | Joback Method |
| vc | 1.139 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

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

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0003257 | Paxs | 543.62 | Joback Method |
| dvisc | 0.0001793 | Paxs | 607.54 | Joback Method |
| dvisc | 0.0001106 | Paxs | 671.47 | Joback Method |
| dvisc | 0.0000742 | Paxs | 735.39 | Joback Method |
| dvisc | 0.0000531 | Paxs | 799.32 | Joback Method |
| dvisc | 0.0000399 | Paxs | 863.24 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U416005&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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 |

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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<https://www.chemeo.com/cid/87-202-1/Terephthalic-acid-4-methylhept-3-yl-pentyl-ester.pdf>

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