

Terephthalic acid, di(4-methylhept-3-yl) ester

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|-----------------------------|--|
| Inchi: | InChI=1S/C24H38O4/c1-7-11-17(5)21(9-3)27-23(25)19-13-15-20(16-14-19)24(26)28-22(|
| InchiKey: | PKPWQVSCJMDEQW-UHFFFAOYSA-N |
| Formula: | C24H38O4 |
| SMILES: | CCCC(C)C(CC)OC(=O)c1ccc(C(=O)OC(CC)C(C)CCC)cc1 |
| Mol. weight [g/mol]: | 390.56 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -223.62 | kJ/mol | Joback Method |
| hf | -824.35 | kJ/mol | Joback Method |
| hfus | 43.05 | kJ/mol | Joback Method |
| hvap | 88.72 | kJ/mol | Joback Method |
| log10ws | -7.56 | | Crippen Method |
| logp | 6.430 | | Crippen Method |
| mcvol | 340.140 | ml/mol | McGowan Method |
| pc | 1052.77 | kPa | Joback Method |
| rinpol | 2138.00 | | NIST Webbook |
| rinpol | 2138.00 | | NIST Webbook |
| tb | 931.00 | K | Joback Method |
| tc | 1143.02 | K | Joback Method |
| tf | 483.50 | K | Joback Method |
| vc | 1.296 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1121.15 | J/molxK | 931.00 | Joback Method |
| cpg | 1192.44 | J/molxK | 1107.68 | Joback Method |
| cpg | 1180.91 | J/molxK | 1072.34 | Joback Method |
| cpg | 1168.06 | J/molxK | 1037.01 | Joback Method |
| cpg | 1153.84 | J/molxK | 1001.67 | Joback Method |
| cpg | 1138.22 | J/molxK | 966.34 | Joback Method |
| cpg | 1202.67 | J/molxK | 1143.02 | Joback Method |
| dvisc | 0.0000213 | Paxs | 931.00 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0000294 | Paxs | 856.42 | Joback Method |
| dvisc | 0.0000432 | Paxs | 781.83 | Joback Method |
| dvisc | 0.0000687 | Paxs | 707.25 | Joback Method |
| dvisc | 0.0001219 | Paxs | 632.67 | Joback Method |
| dvisc | 0.0002520 | Paxs | 558.08 | Joback Method |
| dvisc | 0.0006523 | Paxs | 483.50 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=U416006&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|----------------------------|---|
| cp_g: | 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: | Log ₁₀ 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/86-795-5/Terephthalic-acid-di-4-methylhept-3-yl-ester.pdf>

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