

# Terephthalic acid, heptyl 3-methoxyphenyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C22H26O5/c1-3-4-5-6-7-15-26-21(23)17-11-13-18(14-12-17)22(24)27-20-10-8

WAQMBXCPFSKHJS-UHFFFAOYSA-N

C22H26O5

CCCCCCCOC(=O)c1ccc(C(=O)Oc2cccc(OC)c2)cc1

370.44

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -232.92 | kJ/mol  | Joback Method  |
| hf            | -669.11 | kJ/mol  | Joback Method  |
| hfus          | 46.80   | kJ/mol  | Joback Method  |
| hvap          | 91.16   | kJ/mol  | Joback Method  |
| log10ws       | -6.43   |         | Crippen Method |
| logp          | 5.042   |         | Crippen Method |
| mcvol         | 294.070 | ml/mol  | McGowan Method |
| pc            | 1453.46 | kPa     | Joback Method  |
| rinpol        | 3195.00 |         | NIST Webbook   |
| rinpol        | 3195.00 |         | NIST Webbook   |
| tb            | 941.08  | K       | Joback Method  |
| tc            | 1164.13 | K       | Joback Method  |
| tf            | 582.13  | K       | Joback Method  |
| vc            | 1.117   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 924.20    | J/mol×K | 941.08          | Joback Method |
| cpg           | 937.58    | J/mol×K | 978.26          | Joback Method |
| cpg           | 949.51    | J/mol×K | 1015.43         | Joback Method |
| cpg           | 960.00    | J/mol×K | 1052.61         | Joback Method |
| cpg           | 969.08    | J/mol×K | 1089.78         | Joback Method |
| cpg           | 976.76    | J/mol×K | 1126.96         | Joback Method |
| cpg           | 983.08    | J/mol×K | 1164.13         | Joback Method |
| dvisc         | 0.0002639 | Pa×s    | 582.13          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001580 | Pa×s | 641.95 | Joback Method |
| dvisc | 0.0001032 | Pa×s | 701.78 | Joback Method |
| dvisc | 0.0000721 | Pa×s | 761.61 | Joback Method |
| dvisc | 0.0000531 | Pa×s | 821.43 | Joback Method |
| dvisc | 0.0000407 | Pa×s | 881.25 | Joback Method |
| dvisc | 0.0000323 | Pa×s | 941.08 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U415823&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U415823&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rinpol:</b>  | Non-polar retention indices                     |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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