

# 1,2,3-Propanetriol, tribenzoate

|                      |                                                                                                                                           |
|----------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | Glycerol, tribenzoate<br>Glyceryl tribenzoate<br>Tribenzoin<br>Mollit B<br>Plastic A<br>Uniplex 260<br>2,3-Bis(benzoyloxy)propyl benzoate |
| Inchi:               | InChI=1S/C24H20O6/c25-22(18-10-4-1-5-11-18)28-16-21(30-24(27)20-14-8-3-9-15-20)1                                                          |
| InchiKey:            | HIZCTWCPHWUPFU-UHFFFAOYSA-N                                                                                                               |
| Formula:             | C24H20O6                                                                                                                                  |
| SMILES:              | O=C(OCC(COC(=O)c1ccccc1)OC(=O)c1ccccc1)c1ccccc1                                                                                           |
| Mol. weight [g/mol]: | 404.41                                                                                                                                    |
| CAS:                 | 614-33-5                                                                                                                                  |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -215.77 | kJ/mol  | Joback Method  |
| hf            | -568.78 | kJ/mol  | Joback Method  |
| hfus          | 44.88   | kJ/mol  | Joback Method  |
| hvap          | 102.93  | kJ/mol  | Joback Method  |
| log10ws       | -5.61   |         | Crippen Method |
| logp          | 3.926   |         | Crippen Method |
| mcvol         | 300.060 | ml/mol  | McGowan Method |
| pc            | 1760.97 | kPa     | Joback Method  |
| tb            | 1056.99 | K       | Joback Method  |
| tc            | 1309.45 | K       | Joback Method  |
| tf            | 640.98  | K       | Joback Method  |
| vc            | 1.121   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 966.36 | J/mol×K | 1309.45         | Joback Method |
| cpg           | 965.48 | J/mol×K | 1267.37         | Joback Method |

|       |           |         |         |               |
|-------|-----------|---------|---------|---------------|
| cpg   | 963.23    | J/mol×K | 1225.30 | Joback Method |
| cpg   | 959.55    | J/mol×K | 1183.22 | Joback Method |
| cpg   | 954.36    | J/mol×K | 1141.14 | Joback Method |
| cpg   | 947.60    | J/mol×K | 1099.07 | Joback Method |
| cpg   | 939.18    | J/mol×K | 1056.99 | Joback Method |
| dvisc | 0.0002110 | Pa×s    | 640.98  | Joback Method |
| dvisc | 0.0000203 | Pa×s    | 1056.99 | Joback Method |
| dvisc | 0.0000261 | Pa×s    | 987.65  | Joback Method |
| dvisc | 0.0000350 | Pa×s    | 918.32  | Joback Method |
| dvisc | 0.0000491 | Pa×s    | 848.99  | Joback Method |
| dvisc | 0.0000732 | Pa×s    | 779.65  | Joback Method |
| dvisc | 0.0001181 | Pa×s    | 710.32  | Joback Method |
| hvapt | 123.50    | kJ/mol  | 449.50  | NIST Webbook  |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| <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=C614335&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C614335&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>                         |

## 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>hvapt:</b>   | Enthalpy of vaporization at a given temperature |
| <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>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |

**vc:** Critical Volume

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