

# Phenol, 4-(triphenylmethyl)-

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | p-Cresol, «alpha», «alpha», «alpha»-triphenyl-<br>p-Tritylphenol<br>4-Tritylphenol<br>p-Triphenylmethylphenol |
| <b>Inchi:</b>               | InChI=1S/C25H20O/c26-24-18-16-23(17-19-24)25(20-10-4-1-5-11-20,21-12-6-2-7-13-21                              |
| <b>InchiKey:</b>            | NIPKXTKKYSKEON-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C25H20O   |
| <b>SMILES:</b>              | Oc1ccc(C(c2ccccc2)(c2ccccc2)c2ccccc2)cc1  |
| <b>Mol. weight [g/mol]:</b> | 336.43  |
| <b>CAS:</b>                 | 978-86-9  |

## Physical Properties

| Property code | Value         | Unit    | Source         |
|---------------|---------------|---------|----------------|
| gf            | 457.48        | kJ/mol  | Joback Method  |
| hf            | 200.73        | kJ/mol  | Joback Method  |
| hfus          | 35.04         | kJ/mol  | Joback Method  |
| hvap          | 92.07         | kJ/mol  | Joback Method  |
| log10ws       | -6.23         |         | Crippen Method |
| logp          | 5.775         |         | Crippen Method |
| mcvol         | 273.940       | ml/mol  | McGowan Method |
| pc            | 2212.45       | kPa     | Joback Method  |
| tb            | 955.51        | K       | Joback Method  |
| tc            | 1246.74       | K       | Joback Method  |
| tf            | 555.00 ± 4.00 | K       | NIST Webbook   |
| vc            | 0.959         | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 843.26 | J/molxK | 955.51          | Joback Method |
| cpg           | 860.29 | J/molxK | 1004.05         | Joback Method |
| cpg           | 876.83 | J/molxK | 1052.59         | Joback Method |
| cpg           | 893.29 | J/molxK | 1101.13         | Joback Method |
| cpg           | 910.09 | J/molxK | 1149.66         | Joback Method |

|       |           |         |         |               |
|-------|-----------|---------|---------|---------------|
| cpg   | 927.63    | J/mol×K | 1198.20 | Joback Method |
| cpg   | 946.32    | J/mol×K | 1246.74 | Joback Method |
| dvisc | 0.0000565 | Paxs    | 591.33  | Joback Method |
| dvisc | 0.0000236 | Paxs    | 652.03  | Joback Method |
| dvisc | 0.0000114 | Paxs    | 712.72  | Joback Method |
| dvisc | 0.0000062 | Paxs    | 773.42  | Joback Method |
| dvisc | 0.0000037 | Paxs    | 834.12  | Joback Method |
| dvisc | 0.0000023 | Paxs    | 894.81  | Joback Method |
| dvisc | 0.0000016 | Paxs    | 955.51  | 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=C978869&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C978869&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

Latest version available from:

<https://www.cheméo.com/cid/72-311-6/Phenol-4-triphenylmethyl.pdf>

Generated by Cheméo on 2024-04-29 05:45:59.14167107 +0000 UTC m=+16658808.062248396.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.