

# 1,2,6-triphenyl-3-hexene

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C24H24/c1-4-12-21(13-5-1)14-10-11-19-24(23-17-8-3-9-18-23)20-22-15-6-2-7 |
| <b>InchiKey:</b>            | OIPRUWYSKMFFON-YBFXNURJSA-N   |
| <b>Formula:</b>             | C24H24  |
| <b>SMILES:</b>              | C(=CC(Cc1ccccc1)c1ccccc1)CCc1ccccc1   |
| <b>Mol. weight [g/mol]:</b> | 312.45  |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 566.21  | kJ/mol  | Joback Method  |
| hf            | 282.84  | kJ/mol  | Joback Method  |
| hfus          | 36.72   | kJ/mol  | Joback Method  |
| hvap          | 75.42   | kJ/mol  | Joback Method  |
| log10ws       | -7.00   |         | Crippen Method |
| logp          | 6.202   |         | Crippen Method |
| mcvol         | 273.440 | ml/mol  | McGowan Method |
| pc            | 1640.43 | kPa     | Joback Method  |
| rinpol        | 2513.50 |         | NIST Webbook   |
| rinpol        | 2513.50 |         | NIST Webbook   |
| rinpol        | 2513.50 |         | NIST Webbook   |
| tb            | 832.28  | K       | Joback Method  |
| tc            | 1081.71 | K       | Joback Method  |
| tf            | 419.42  | K       | Joback Method  |
| vc            | 1.030   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 805.16 | J/molxK | 832.28          | Joback Method |
| cpg           | 885.20 | J/molxK | 1040.14         | Joback Method |
| cpg           | 871.40 | J/molxK | 998.57          | Joback Method |
| cpg           | 856.67 | J/molxK | 956.99          | Joback Method |
| cpg           | 840.84 | J/molxK | 915.42          | Joback Method |
| cpg           | 823.72 | J/molxK | 873.85          | Joback Method |
| cpg           | 898.23 | J/molxK | 1081.71         | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0000492 | Paxs | 832.28 | Joback Method |
| dvisc | 0.0000658 | Paxs | 763.47 | Joback Method |
| dvisc | 0.0000932 | Paxs | 694.66 | Joback Method |
| dvisc | 0.0001425 | Paxs | 625.85 | Joback Method |
| dvisc | 0.0002421 | Paxs | 557.04 | Joback Method |
| dvisc | 0.0004775 | Paxs | 488.23 | Joback Method |
| dvisc | 0.0011770 | Paxs | 419.42 | 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=R316019&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R316019&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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