

# Benzene, 1,1',1''-ethyldynetris-

|                      |                                                                                    |
|----------------------|------------------------------------------------------------------------------------|
| Other names:         | Ethane, 1,1,1-triphenyl-<br>1,1,1-Triphenylethane                                  |
| Inchi:               | InChI=1S/C20H18/c1-20(17-11-5-2-6-12-17,18-13-7-3-8-14-18)19-15-9-4-10-16-19/h2-16 |
| InchiKey:            | QIDUHGHEFWAMMPV-UHFFFAOYSA-N                                                       |
| Formula:             | C20H18                                                                             |
| SMILES:              | CC(c1ccccc1)(c1ccccc1)c1ccccc1                                                     |
| Mol. weight [g/mol]: | 258.36                                                                             |
| CAS:                 | 5271-39-6                                                                          |

## Physical Properties

| Property code | Value         | Unit    | Source         |
|---------------|---------------|---------|----------------|
| gf            | 457.59        | kJ/mol  | Joback Method  |
| hf            | 244.71        | kJ/mol  | Joback Method  |
| hfus          | 22.27         | kJ/mol  | Joback Method  |
| hvap          | 65.65         | kJ/mol  | Joback Method  |
| log10ws       | -5.38         |         | Crippen Method |
| logp          | 5.041         |         | Crippen Method |
| mcvol         | 221.380       | ml/mol  | McGowan Method |
| pc            | 2212.45       | kPa     | Joback Method  |
| tb            | 733.81        | K       | Joback Method  |
| tc            | 1006.17       | K       | Joback Method  |
| tf            | 367.40 ± 0.60 | K       | NIST Webbook   |
| tf            | 367.60 ± 2.00 | K       | NIST Webbook   |
| tf            | 368.05 ± 0.30 | K       | NIST Webbook   |
| tf            | 367.45 ± 0.20 | K       | NIST Webbook   |
| tf            | 366.00 ± 4.00 | K       | NIST Webbook   |
| tf            | 367.90 ± 3.00 | K       | NIST Webbook   |
| vc            | 0.821         | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 606.48 | J/mol×K | 733.81          | Joback Method |
| cpg           | 625.80 | J/mol×K | 779.20          | Joback Method |

|       |           |         |         |               |
|-------|-----------|---------|---------|---------------|
| cpg   | 643.25    | J/mol×K | 824.60  | Joback Method |
| cpg   | 659.05    | J/mol×K | 869.99  | Joback Method |
| cpg   | 673.41    | J/mol×K | 915.38  | Joback Method |
| cpg   | 686.53    | J/mol×K | 960.78  | Joback Method |
| cpg   | 698.63    | J/mol×K | 1006.17 | Joback Method |
| dvisc | 0.0015538 | Pa×s    | 396.84  | Joback Method |
| dvisc | 0.0007039 | Pa×s    | 453.00  | Joback Method |
| dvisc | 0.0003798 | Pa×s    | 509.16  | Joback Method |
| dvisc | 0.0002316 | Pa×s    | 565.33  | Joback Method |
| dvisc | 0.0001545 | Pa×s    | 621.49  | Joback Method |
| dvisc | 0.0001102 | Pa×s    | 677.65  | Joback Method |
| dvisc | 0.0000827 | Pa×s    | 733.81  | Joback Method |

## Sources

|                        |                                                                                                                                             |
|------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| <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>                                       |
| <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=C5271396&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5271396&amp;Units=SI</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                                 |

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