

# Triphenylene, octadecahydro-

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | octadecahydrotriphenylene   |
| <b>Inchi:</b>               | InChI=1S/C18H30/c1-2-8-14-13(7-1)15-9-3-4-11-17(15)18-12-6-5-10-16(14)18/h13-18H, |
| <b>InchiKey:</b>            | GSCVIAUUCUEVEH-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C18H30  |
| <b>SMILES:</b>              | C1CCC2C(C1)C1CCCCC1C1CCCCC21  |
| <b>Mol. weight [g/mol]:</b> | 246.43  |
| <b>CAS:</b>                 | 15074-91-6  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 255.66  | kJ/mol               | Joback Method  |
| hf            | -201.29 | kJ/mol               | Joback Method  |
| hfus          | 24.46   | kJ/mol               | Joback Method  |
| hvap          | 55.73   | kJ/mol               | Joback Method  |
| log10ws       | -5.49   |                      | Crippen Method |
| logp          | 5.419   |                      | Crippen Method |
| mcvol         | 221.040 | ml/mol               | McGowan Method |
| pc            | 1823.17 | kPa                  | Joback Method  |
| tb            | 654.48  | K                    | Joback Method  |
| tc            | 892.74  | K                    | Joback Method  |
| tf            | 334.78  | K                    | Joback Method  |
| vc            | 0.822   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 693.36    | J/molxK | 654.48          | Joback Method |
| cpg           | 723.24    | J/molxK | 694.19          | Joback Method |
| cpg           | 750.96    | J/molxK | 733.90          | Joback Method |
| cpg           | 776.64    | J/molxK | 773.61          | Joback Method |
| cpg           | 800.42    | J/molxK | 813.32          | Joback Method |
| cpg           | 822.44    | J/molxK | 853.03          | Joback Method |
| cpg           | 842.84    | J/molxK | 892.74          | Joback Method |
| dvisc         | 0.0037204 | Paxs    | 334.78          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0027614 | Paxs | 388.06 | Joback Method |
| dvisc | 0.0022026 | Paxs | 441.35 | Joback Method |
| dvisc | 0.0018446 | Paxs | 494.63 | Joback Method |
| dvisc | 0.0015990 | Paxs | 547.91 | Joback Method |
| dvisc | 0.0014216 | Paxs | 601.20 | Joback Method |
| dvisc | 0.0012884 | Paxs | 654.48 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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.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=C15074916&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C15074916&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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