

# 1,3-di-isobutylmesitylene

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C17H28/c1-11(2)8-16-13(5)10-14(6)17(15(16)7)9-12(3)4/h10-12H,8-9H2,1-7H1 |
| <b>InchiKey:</b>            | JOQYFRRUSWTDQJ-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C17H28  |
| <b>SMILES:</b>              | <chem>Cc1cc(C)c(CC(C)C)c(C)c1CC(C)C</chem>  |
| <b>Mol. weight [g/mol]:</b> | 232.40  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 161.27  | kJ/mol               | Joback Method  |
| hf            | -214.12 | kJ/mol               | Joback Method  |
| hfus          | 25.22   | kJ/mol               | Joback Method  |
| hvap          | 57.58   | kJ/mol               | Joback Method  |
| log10ws       | -5.70   |                      | Crippen Method |
| logp          | 5.009   |                      | Crippen Method |
| mvol          | 226.630 | ml/mol               | McGowan Method |
| pc            | 1522.31 | kPa                  | Joback Method  |
| rinpol        | 1640.00 |                      | NIST Webbook   |
| rinpol        | 1640.00 |                      | NIST Webbook   |
| tb            | 634.08  | K                    | Joback Method  |
| tc            | 831.82  | K                    | Joback Method  |
| tf            | 327.85  | K                    | Joback Method  |
| vc            | 0.868   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 600.46    | J/mol×K | 634.08          | Joback Method |
| cpg           | 619.86    | J/mol×K | 667.04          | Joback Method |
| cpg           | 638.32    | J/mol×K | 699.99          | Joback Method |
| cpg           | 655.84    | J/mol×K | 732.95          | Joback Method |
| cpg           | 672.47    | J/mol×K | 765.90          | Joback Method |
| cpg           | 688.22    | J/mol×K | 798.86          | Joback Method |
| cpg           | 703.11    | J/mol×K | 831.82          | Joback Method |
| dvisc         | 0.0016354 | Paxs    | 327.85          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0007757 | Paxs | 378.89 | Joback Method |
| dvisc | 0.0004393 | Paxs | 429.93 | Joback Method |
| dvisc | 0.0002806 | Paxs | 480.96 | Joback Method |
| dvisc | 0.0001954 | Paxs | 532.00 | Joback Method |
| dvisc | 0.0001449 | Paxs | 583.04 | Joback Method |
| dvisc | 0.0001128 | Paxs | 634.08 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R200776&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R200776&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.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>                     |

## 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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