

# 1-Isopropyl-3,5-di-n-Propylbenzene

|                      |                                                                            |
|----------------------|----------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C15H24/c1-5-7-13-9-14(8-6-2)11-15(10-13)12(3)4/h9-12H,5-8H2,1-4H3 |
| InchiKey:            | PBFVIHCLUVKHFV-UHFFFAOYSA-N                                                |
| Formula:             | C15H24                                                                     |
| SMILES:              | CCCC1cc(CCC)cc(C(C)C)c1                                                    |
| Mol. weight [g/mol]: | 204.35                                                                     |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 166.13  | kJ/mol  | Joback Method  |
| hf            | -144.62 | kJ/mol  | Joback Method  |
| hfus          | 24.35   | kJ/mol  | Joback Method  |
| hvap          | 52.20   | kJ/mol  | Joback Method  |
| log10ws       | -5.10   |         | Crippen Method |
| logp          | 4.715   |         | Crippen Method |
| mcvol         | 198.450 | ml/mol  | McGowan Method |
| pc            | 1812.32 | kPa     | Joback Method  |
| ripol         | 1564.00 |         | NIST Webbook   |
| ripol         | 1563.60 |         | NIST Webbook   |
| ripol         | 1564.00 |         | NIST Webbook   |
| tb            | 578.80  | K       | Joback Method  |
| tc            | 776.15  | K       | Joback Method  |
| tf            | 295.27  | K       | Joback Method  |
| vc            | 0.761   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 493.80 | J/mol×K | 578.80          | Joback Method |
| cpg           | 577.53 | J/mol×K | 743.26          | Joback Method |
| cpg           | 562.52 | J/mol×K | 710.37          | Joback Method |
| cpg           | 546.68 | J/mol×K | 677.48          | Joback Method |
| cpg           | 529.97 | J/mol×K | 644.58          | Joback Method |
| cpg           | 512.35 | J/mol×K | 611.69          | Joback Method |
| cpg           | 591.72 | J/mol×K | 776.15          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001485 | Pa×s | 578.80 | Joback Method |
| dvisc | 0.0001926 | Pa×s | 531.54 | Joback Method |
| dvisc | 0.0002628 | Pa×s | 484.29 | Joback Method |
| dvisc | 0.0003833 | Pa×s | 437.03 | Joback Method |
| dvisc | 0.0006129 | Pa×s | 389.78 | Joback Method |
| dvisc | 0.0011153 | Pa×s | 342.52 | Joback Method |
| dvisc | 0.0024583 | Pa×s | 295.27 | 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=R305683&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R305683&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>ripol:</b>   | 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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