

# cis-3-Isopropylhexa-1,4-diene

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C9H16/c1-5-7-9(6-2)8(3)4/h5-9H,2H2,1,3-4H3/b7-5- |
| <b>InchiKey:</b>            | WUHBPVXKLJAZIG-ALCCZGGFSA-N                               |
| <b>Formula:</b>             | C9H16   |
| <b>SMILES:</b>              | C=CC(C=CC)C(C)C   |
| <b>Mol. weight [g/mol]:</b> | 124.22  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 188.08  | kJ/mol               | Joback Method  |
| hf            | 3.00    | kJ/mol               | Joback Method  |
| hfus          | 10.94   | kJ/mol               | Joback Method  |
| hvap          | 34.14   | kJ/mol               | Joback Method  |
| log10ws       | -2.81   |                      | Crippen Method |
| logp          | 3.021   |                      | Crippen Method |
| mcvol         | 129.070 | ml/mol               | McGowan Method |
| pc            | 2571.50 | kPa                  | Joback Method  |
| ripol         | 947.00  |                      | NIST Webbook   |
| ripol         | 947.00  |                      | NIST Webbook   |
| tb            | 405.28  | K                    | Joback Method  |
| tc            | 588.15  | K                    | Joback Method  |
| tf            | 154.35  | K                    | Joback Method  |
| vc            | 0.488   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 242.58    | J/mol×K | 405.28          | Joback Method |
| cpg           | 307.37    | J/mol×K | 557.67          | Joback Method |
| cpg           | 295.68    | J/mol×K | 527.20          | Joback Method |
| cpg           | 283.38    | J/mol×K | 496.72          | Joback Method |
| cpg           | 270.45    | J/mol×K | 466.24          | Joback Method |
| cpg           | 256.86    | J/mol×K | 435.76          | Joback Method |
| cpg           | 318.49    | J/mol×K | 588.15          | Joback Method |
| dvisc         | 0.0001834 | Paxs    | 405.28          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0002539 | Paxs | 363.46 | Joback Method |
| dvisc | 0.0003823 | Paxs | 321.64 | Joback Method |
| dvisc | 0.0006508 | Paxs | 279.81 | Joback Method |
| dvisc | 0.0013354 | Paxs | 237.99 | Joback Method |
| dvisc | 0.0037231 | Paxs | 196.17 | Joback Method |
| dvisc | 0.0180922 | Paxs | 154.35 | 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=R237540&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R237540&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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