

# 1H-Indene, 1-phenylmethyl

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C16H14/c1-2-6-13(7-3-1)12-15-11-10-14-8-4-5-9-16(14)15/h1-11,15H,12H2 |
| <b>InchiKey:</b>            | NBHBNYRLTADHQY-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C16H14   |
| <b>SMILES:</b>              | C1=CC(Cc2ccccc2)c2ccccc21  |
| <b>Mol. weight [g/mol]:</b> | 206.28   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 389.74  | kJ/mol  | Joback Method  |
| hf            | 218.60  | kJ/mol  | Joback Method  |
| hfus          | 24.25   | kJ/mol  | Joback Method  |
| hvap          | 56.63   | kJ/mol  | Joback Method  |
| log10ws       | -4.57   |         | Crippen Method |
| logp          | 4.040   |         | Crippen Method |
| mcvol         | 173.620 | ml/mol  | McGowan Method |
| pc            | 2654.29 | kPa     | Joback Method  |
| rinpol        | 1892.00 |         | NIST Webbook   |
| tb            | 629.72  | K       | Joback Method  |
| tc            | 880.12  | K       | Joback Method  |
| tf            | 354.14  | K       | Joback Method  |
| vc            | 0.658   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 435.82    | J/molxK | 629.72          | Joback Method |
| cpg           | 453.69    | J/molxK | 671.45          | Joback Method |
| cpg           | 470.07    | J/molxK | 713.19          | Joback Method |
| cpg           | 485.09    | J/molxK | 754.92          | Joback Method |
| cpg           | 498.90    | J/molxK | 796.65          | Joback Method |
| cpg           | 511.62    | J/molxK | 838.39          | Joback Method |
| cpg           | 523.39    | J/molxK | 880.12          | Joback Method |
| dvisc         | 0.0017311 | Paxs    | 354.14          | Joback Method |
| dvisc         | 0.0011653 | Paxs    | 400.07          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0008510 | Paxs | 446.00 | Joback Method |
| dvisc | 0.0006591 | Paxs | 491.93 | Joback Method |
| dvisc | 0.0005332 | Paxs | 537.86 | Joback Method |
| dvisc | 0.0004460 | Paxs | 583.79 | Joback Method |
| dvisc | 0.0003829 | Paxs | 629.72 | 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=R72945&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R72945&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>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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