

# Indane, 1-methyl-3-phenyl-

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | 1H-Indene, 2,3-dihydro-1-methyl-3-phenyl-1-methyl-3-phenylindan                   |
| <b>Inchi:</b>               | InChI=1S/C16H16/c1-12-11-16(13-7-3-2-4-8-13)15-10-6-5-9-14(12)15/h2-10,12,16H,11H |
| <b>InchiKey:</b>            | JHIDJKSBZPNVKZ-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C16H16  |
| <b>SMILES:</b>              | CC1CC(c2ccccc2)c2ccccc21  |
| <b>Mol. weight [g/mol]:</b> | 208.30  |
| <b>CAS:</b>                 | 6416-39-3   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 352.07  | kJ/mol  | Joback Method  |
| hf            | 140.48  | kJ/mol  | Joback Method  |
| hfus          | 24.10   | kJ/mol  | Joback Method  |
| hvap          | 56.03   | kJ/mol  | Joback Method  |
| log10ws       | -4.62   |         | Crippen Method |
| logp          | 4.326   |         | Crippen Method |
| mcvol         | 177.920 | ml/mol  | McGowan Method |
| pc            | 2475.19 | kPa     | Joback Method  |
| rinpol        | 1675.00 |         | NIST Webbook   |
| rinpol        | 1660.00 |         | NIST Webbook   |
| tb            | 625.89  | K       | Joback Method  |
| tc            | 873.99  | K       | Joback Method  |
| tf            | 349.14  | K       | Joback Method  |
| vc            | 0.671   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 459.51 | J/molxK | 625.89          | Joback Method |
| cpg           | 479.19 | J/molxK | 667.24          | Joback Method |
| cpg           | 497.31 | J/molxK | 708.59          | Joback Method |
| cpg           | 514.00 | J/molxK | 749.94          | Joback Method |
| cpg           | 529.38 | J/molxK | 791.29          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 543.55    | J/molxK | 832.64 | Joback Method |
| cpg   | 556.64    | J/molxK | 873.99 | Joback Method |
| dvisc | 0.0016648 | Paxs    | 349.14 | Joback Method |
| dvisc | 0.0011646 | Paxs    | 395.26 | Joback Method |
| dvisc | 0.0008779 | Paxs    | 441.39 | Joback Method |
| dvisc | 0.0006981 | Paxs    | 487.51 | Joback Method |
| dvisc | 0.0005776 | Paxs    | 533.64 | Joback Method |
| dvisc | 0.0004925 | Paxs    | 579.76 | Joback Method |
| dvisc | 0.0004299 | Paxs    | 625.89 | 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=C6416393&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6416393&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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