

# Indene

|                      |                                                |
|----------------------|------------------------------------------------|
| Other names:         | 1H-Indene<br>INDEN<br>INDONAPHTHENE            |
| Inchi:               | InChI=1S/C9H8/c1-2-5-9-7-3-6-8(9)4-1/h1-6H,7H2 |
| InchiKey:            | YBYIRNPNPPLQARY-UHFFFAOYSA-N                   |
| Formula:             | C9H8                                           |
| SMILES:              | C1=Cc2ccccc2C1                                 |
| Mol. weight [g/mol]: | 116.16                                         |
| CAS:                 | 95-13-6                                        |

## Physical Properties

| Property code | Value           | Unit   | Source         |
|---------------|-----------------|--------|----------------|
| af            | 0.2620          |        | KDB            |
| affp          | 848.50          | kJ/mol | NIST Webbook   |
| affp          | 848.80          | kJ/mol | NIST Webbook   |
| basg          | 819.60          | kJ/mol | NIST Webbook   |
| basg          | 819.20          | kJ/mol | NIST Webbook   |
| chl           | -4795.50 ± 1.30 | kJ/mol | NIST Webbook   |
| ea            | 0.17 ± 0.03     | eV     | NIST Webbook   |
| gf            | 226.10          | kJ/mol | Joback Method  |
| hf            | 161.20 ± 2.30   | kJ/mol | NIST Webbook   |
| hfl           | 110.60 ± 1.80   | kJ/mol | NIST Webbook   |
| hfl           | 110.00 ± 1.00   | kJ/mol | NIST Webbook   |
| hfus          | 11.00           | kJ/mol | Joback Method  |
| hvap          | 50.60 ± 1.50    | kJ/mol | NIST Webbook   |
| ie            | 8.33 ± 0.01     | eV     | NIST Webbook   |
| ie            | 8.15 ± 0.01     | eV     | NIST Webbook   |
| ie            | 8.13 ± 0.05     | eV     | NIST Webbook   |
| ie            | 8.62            | eV     | NIST Webbook   |
| ie            | 8.14 ± 0.01     | eV     | NIST Webbook   |
| ie            | 8.14 ± 0.01     | eV     | NIST Webbook   |
| log10ws       | -2.57           |        | Crippen Method |
| logp          | 2.256           |        | Crippen Method |
| mcvol         | 98.750          | ml/mol | McGowan Method |
| pc            | 3800.00         | kPa    | KDB            |
| rinpol        | 1025.00         |        | NIST Webbook   |
| rinpol        | 1015.70         |        | NIST Webbook   |

|        |         |              |
|--------|---------|--------------|
| rinpol | 1034.10 | NIST Webbook |
| rinpol | 1043.30 | NIST Webbook |
| rinpol | 1053.80 | NIST Webbook |
| rinpol | 1021.00 | NIST Webbook |
| rinpol | 1011.80 | NIST Webbook |
| rinpol | 1011.80 | NIST Webbook |
| rinpol | 1016.90 | NIST Webbook |
| rinpol | 1016.90 | NIST Webbook |
| rinpol | 1017.00 | NIST Webbook |
| rinpol | 1017.50 | NIST Webbook |
| rinpol | 1060.00 | NIST Webbook |
| rinpol | 1030.00 | NIST Webbook |
| rinpol | 1062.00 | NIST Webbook |
| rinpol | 1026.00 | NIST Webbook |
| rinpol | 1037.00 | NIST Webbook |
| rinpol | 1072.50 | NIST Webbook |
| rinpol | 1069.00 | NIST Webbook |
| rinpol | 1041.00 | NIST Webbook |
| rinpol | 1045.00 | NIST Webbook |
| rinpol | 1054.00 | NIST Webbook |
| rinpol | 1011.00 | NIST Webbook |
| rinpol | 1014.00 | NIST Webbook |
| rinpol | 1036.00 | NIST Webbook |
| rinpol | 1033.00 | NIST Webbook |
| rinpol | 1051.00 | NIST Webbook |
| rinpol | 1049.00 | NIST Webbook |
| rinpol | 1039.00 | NIST Webbook |
| rinpol | 1023.00 | NIST Webbook |
| rinpol | 1024.00 | NIST Webbook |
| rinpol | 1025.00 | NIST Webbook |
| rinpol | 1042.00 | NIST Webbook |
| rinpol | 1036.00 | NIST Webbook |
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| rinpol | 1041.00 | NIST Webbook |
| rinpol | 1059.00 | NIST Webbook |
| rinpol | 1031.00 | NIST Webbook |
| rinpol | 1059.00 | NIST Webbook |
| rinpol | 1020.00 | NIST Webbook |
| rinpol | 1042.00 | NIST Webbook |
| rinpol | 1045.00 | NIST Webbook |
| rinpol | 1017.00 | NIST Webbook |
| rinpol | 1059.00 | NIST Webbook |
| rinpol | 1062.00 | NIST Webbook |

|        |         |              |
|--------|---------|--------------|
| rinpol | 171.05  | NIST Webbook |
| rinpol | 173.26  | NIST Webbook |
| rinpol | 172.05  | NIST Webbook |
| rinpol | 172.51  | NIST Webbook |
| rinpol | 170.83  | NIST Webbook |
| rinpol | 169.00  | NIST Webbook |
| rinpol | 168.80  | NIST Webbook |
| rinpol | 170.08  | NIST Webbook |
| rinpol | 169.00  | NIST Webbook |
| rinpol | 171.05  | NIST Webbook |
| rinpol | 1060.00 | NIST Webbook |
| rinpol | 1059.00 | NIST Webbook |
| rinpol | 1016.00 | NIST Webbook |
| rinpol | 1031.00 | NIST Webbook |
| rinpol | 1023.30 | NIST Webbook |
| rinpol | 1011.80 | NIST Webbook |
| rinpol | 1021.00 | NIST Webbook |
| rinpol | 1017.00 | NIST Webbook |
| rinpol | 1049.00 | NIST Webbook |
| rinpol | 1059.00 | NIST Webbook |
| rinpol | 1023.30 | NIST Webbook |
| rinpol | 1013.00 | NIST Webbook |
| rinpol | 1018.00 | NIST Webbook |
| rinpol | 1026.00 | NIST Webbook |
| rinpol | 1035.00 | NIST Webbook |
| rinpol | 1034.00 | NIST Webbook |
| rinpol | 1031.00 | NIST Webbook |
| rinpol | 1034.00 | NIST Webbook |
| rinpol | 1034.00 | NIST Webbook |
| rinpol | 1016.00 | NIST Webbook |
| rinpol | 1015.00 | NIST Webbook |
| rinpol | 1036.00 | NIST Webbook |
| rinpol | 1059.00 | NIST Webbook |
| rinpol | 1052.00 | NIST Webbook |
| rinpol | 1059.00 | NIST Webbook |
| rinpol | 1031.00 | NIST Webbook |
| rinpol | 1037.00 | NIST Webbook |
| rinpol | 1015.70 | NIST Webbook |
| ripol  | 1431.00 | NIST Webbook |
| ripol  | 1455.80 | NIST Webbook |
| ripol  | 1430.80 | NIST Webbook |
| ripol  | 1479.00 | NIST Webbook |
| ripol  | 1467.00 | NIST Webbook |
| ripol  | 1472.00 | NIST Webbook |

|       |               |         |              |
|-------|---------------|---------|--------------|
| ripol | 1466.00       |         | NIST Webbook |
| ripol | 1471.00       |         | NIST Webbook |
| sl    | 215.35        | J/mol×K | NIST Webbook |
| sl    | 214.18        | J/mol×K | NIST Webbook |
| tb    | 455.59        | K       | KDB          |
| tc    | 695.15        | K       | KDB          |
| tf    | 270.48 ± 0.30 | K       | NIST Webbook |
| tf    | 271.00        | K       | KDB          |
| tf    | 271.40 ± 0.50 | K       | NIST Webbook |
| tt    | 271.70 ± 0.02 | K       | NIST Webbook |
| vc    | 0.368         | m3/kmol | KDB          |
| zc    | 0.2422730     |         | KDB          |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 185.13    | J/mol×K | 447.55          | Joback Method |
| cpg           | 198.30    | J/mol×K | 485.80          | Joback Method |
| cpg           | 210.42    | J/mol×K | 524.05          | Joback Method |
| cpg           | 221.55    | J/mol×K | 562.31          | Joback Method |
| cpg           | 231.79    | J/mol×K | 600.56          | Joback Method |
| cpg           | 241.21    | J/mol×K | 638.81          | Joback Method |
| cpg           | 249.87    | J/mol×K | 677.06          | Joback Method |
| cpl           | 186.94    | J/mol×K | 298.15          | NIST Webbook  |
| cpl           | 186.94    | J/mol×K | 298.15          | NIST Webbook  |
| dvisc         | 0.0003712 | Pa×s    | 447.55          | Joback Method |
| dvisc         | 0.0009934 | Pa×s    | 285.48          | Joback Method |
| dvisc         | 0.0007529 | Pa×s    | 317.90          | Joback Method |
| dvisc         | 0.0014072 | Pa×s    | 253.07          | Joback Method |
| dvisc         | 0.0004979 | Pa×s    | 382.72          | Joback Method |
| dvisc         | 0.0004250 | Pa×s    | 415.14          | Joback Method |
| dvisc         | 0.0006007 | Pa×s    | 350.31          | Joback Method |
| hfust         | 10.20     | kJ/mol  | 271.70          | NIST Webbook  |
| hfust         | 10.20     | kJ/mol  | 271.70          | NIST Webbook  |
| hfust         | 10.20     | kJ/mol  | 271.70          | NIST Webbook  |
| hvapt         | 45.30     | kJ/mol  | 413.00          | NIST Webbook  |
| hvapt         | 43.60     | kJ/mol  | 372.00          | NIST Webbook  |
| hvapt         | 43.90     | kJ/mol  | 391.50          | NIST Webbook  |
| rfi           | 1.57370   |         | 298.15          | KDB           |
| rhoI          | 998.99    | kg/m3   | 293.10          | KDB           |
| sfust         | 37.55     | J/mol×K | 271.70          | NIST Webbook  |

# Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.67872e+01                   |
| Coeff. B                    | -5.48854e+03                  |
| Coeff. C                    | -2.97000e+00                  |
| Temperature range (K), min. | 335.62                        |
| Temperature range (K), max. | 481.24                        |

| Information                 | Value                                                  |
|-----------------------------|--------------------------------------------------------|
| Property code               | pvap                                                   |
| Equation                    | $\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$ |
| Coeff. A                    | 1.22605e+02                                            |
| Coeff. B                    | -1.05135e+04                                           |
| Coeff. C                    | -1.58068e+01                                           |
| Coeff. D                    | 9.00394e-06                                            |
| Temperature range (K), min. | 271.70                                                 |
| Temperature range (K), max. | 693.15                                                 |

## Sources

**The Yaws Handbook of Vapor**

**Pressure:**

**Joback Method:**

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C95136&Units=SI>

**KDB Vapor Pressure Data:**

<https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=750>

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

**Liquid-Liquid Equilibrium**

**Measurements for Model Systems**

**Related to Catalytic Fast Pyrolysis of**

**Biomass:**

<https://www.doi.org/10.1021/acs.jced.6b00625>

[https://www.chemed.com/doc/models/crippen\\_log10ws](https://www.chemed.com/doc/models/crippen_log10ws)

<https://www.thermo.com/files/research/kdb/mol/mol750.mol>

# Legend

|                 |                                                           |
|-----------------|-----------------------------------------------------------|
| <b>af:</b>      | Acentric Factor                                           |
| <b>affp:</b>    | Proton affinity                                           |
| <b>basg:</b>    | Gas basicity                                              |
| <b>chl:</b>     | Standard liquid enthalpy of combustion                    |
| <b>cpg:</b>     | Ideal gas heat capacity                                   |
| <b>cpl:</b>     | Liquid phase heat capacity                                |
| <b>dvisc:</b>   | Dynamic viscosity                                         |
| <b>ea:</b>      | Electron affinity                                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation                   |
| <b>hf:</b>      | Enthalpy of formation at standard conditions              |
| <b>hfl:</b>     | Liquid phase enthalpy of formation at standard conditions |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions                 |
| <b>hfust:</b>   | Enthalpy of fusion at a given temperature                 |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions           |
| <b>hvapt:</b>   | Enthalpy of vaporization at a given temperature           |
| <b>ie:</b>      | Ionization energy                                         |
| <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>pvap:</b>    | Vapor pressure                                            |
| <b>rfi:</b>     | Refractive Index                                          |
| <b>rho:</b>     | Liquid Density                                            |
| <b>rinpol:</b>  | Non-polar retention indices                               |
| <b>ripol:</b>   | Polar retention indices                                   |
| <b>sfust:</b>   | Entropy of fusion at a given temperature                  |
| <b>sl:</b>      | Liquid phase molar entropy at standard conditions         |
| <b>tb:</b>      | Normal Boiling Point Temperature                          |
| <b>tc:</b>      | Critical Temperature                                      |
| <b>tf:</b>      | Normal melting (fusion) point                             |
| <b>tt:</b>      | Triple Point Temperature                                  |
| <b>vc:</b>      | Critical Volume                                           |
| <b>zc:</b>      | Critical Compressibility                                  |

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