

# 1H-INDENE, 2,3-DIMETHYL-

|                      |                                                               |
|----------------------|---------------------------------------------------------------|
| Inchi:               | InChI=1S/C11H12/c1-8-7-10-5-3-4-6-11(10)9(8)2/h3-6H,7H2,1-2H3 |
| InchiKey:            | CXLNYETYUQMZKI-UHFFFAOYSA-N                                   |
| Formula:             | C11H12                                                        |
| SMILES:              | CC1=C(C)c2ccccc2C1                                            |
| Mol. weight [g/mol]: | 144.22                                                        |

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| hf            | 169.44  | kJ/mol | Cheméo Relay (1.0) |
| hfus          | 15.41   | kJ/mol | Joback Method      |
| hvap          | 57.50   | kJ/mol | Cheméo Relay (1.0) |
| ie            | 7.88    | eV     | Cheméo Relay (1.0) |
| log10ws       | -3.44   |        | Cheméo Relay (1.0) |
| logp          | 3.036   |        | Crippen Method     |
| mcvol         | 126.930 | ml/mol | McGowan Method     |
| tb            | 501.92  | K      | Cheméo Relay (1.0) |
| tc            | 724.01  | K      | Cheméo Relay (1.0) |
| tf            | 280.98  | K      | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 269.58    | J/mol×K | 503.27          | Joback Method |
| cpg           | 283.86    | J/mol×K | 540.73          | Joback Method |
| cpg           | 297.19    | J/mol×K | 578.19          | Joback Method |
| cpg           | 309.63    | J/mol×K | 615.65          | Joback Method |
| cpg           | 321.25    | J/mol×K | 653.11          | Joback Method |
| cpg           | 332.10    | J/mol×K | 690.57          | Joback Method |
| cpg           | 342.25    | J/mol×K | 728.03          | Joback Method |
| dvisc         | 0.0011595 | Pa×s    | 300.65          | Joback Method |
| dvisc         | 0.0008680 | Pa×s    | 334.42          | Joback Method |
| dvisc         | 0.0006853 | Pa×s    | 368.19          | Joback Method |
| dvisc         | 0.0005629 | Pa×s    | 401.96          | Joback Method |
| dvisc         | 0.0004767 | Pa×s    | 435.73          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0004135 | Pa×s | 469.50 | Joback Method |
| dvisc | 0.0003656 | Pa×s | 503.27 | Joback Method |

## Sources

|                           |                                                                                                                                             |
|---------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method:           | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |
| Cheméo Relay (1.0):       |                                                                                                                                             |
| Cheméo Relay (1.0, beta): |                                                                                                                                             |
| NIST Webbook:             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4773824&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4773824&amp;Units=SI</a> |
| Joback Method:            | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                       |
| McGowan Method:           | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |
| Crippen Method:           | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                   |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <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>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>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |

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