

# 1-Ethyl-2-methylcyclopentene

|                      |                                                                 |
|----------------------|-----------------------------------------------------------------|
| Other names:         | 1-Ethyl-2-methylcyclopentene<br>Cyclopentene, 1-ethyl-2-methyl- |
| Inchi:               | InChI=1S/C8H14/c1-3-8-6-4-5-7(8)2/h3-6H2,1-2H3                  |
| InchiKey:            | MMYZGQDXYZNAQW-UHFFFAOYSA-N                                     |
| Formula:             | C8H14                                                           |
| SMILES:              | CCC1=C(C)CCC1                                                   |
| Mol. weight [g/mol]: | 110.20                                                          |

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| hf            | -35.77  | kJ/mol | Cheméo Relay (1.0) |
| hfus          | 9.78    | kJ/mol | Joback Method      |
| logp          | 2.897   |        | Crippen Method     |
| mcvol         | 108.420 | ml/mol | McGowan Method     |
| tb            | 400.80  | K      | Cheméo Relay (1.0) |
| tf            | 186.23  | K      | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 204.62    | J/mol×K | 411.51          | Joback Method |
| cpg           | 278.81    | J/mol×K | 609.80          | Joback Method |
| cpg           | 267.96    | J/mol×K | 576.75          | Joback Method |
| cpg           | 256.53    | J/mol×K | 543.70          | Joback Method |
| cpg           | 244.51    | J/mol×K | 510.65          | Joback Method |
| cpg           | 231.87    | J/mol×K | 477.61          | Joback Method |
| cpg           | 218.58    | J/mol×K | 444.56          | Joback Method |
| dvisc         | 0.0005711 | Pa×s    | 316.19          | Joback Method |
| dvisc         | 0.0002697 | Pa×s    | 411.51          | Joback Method |
| dvisc         | 0.0003321 | Pa×s    | 379.74          | Joback Method |
| dvisc         | 0.0004249 | Pa×s    | 347.96          | Joback Method |
| dvisc         | 0.0023108 | Pa×s    | 220.86          | Joback Method |
| dvisc         | 0.0008200 | Pa×s    | 284.41          | Joback Method |
| dvisc         | 0.0012898 | Pa×s    | 252.64          | Joback Method |

# Sources

|                                  |                                                                                                                                               |
|----------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Crippen Method:</b>           | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>Cheméo Relay (1.0):</b>       |                                                                                                                                               |
| <b>Cheméo Relay (1.0, beta):</b> |                                                                                                                                               |
| <b>NIST Webbook:</b>             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C19780564&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C19780564&amp;Units=SI</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>                         |

# 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>logp:</b>  | Octanol/Water partition coefficient          |
| <b>mcvol:</b> | McGowan's characteristic volume              |
| <b>tb:</b>    | Normal Boiling Point Temperature             |
| <b>tf:</b>    | Normal melting (fusion) point                |

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