

# (trans-4,5-Methylenehexyl)-cyclopropane

|                      |                                                                          |
|----------------------|--------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C10H18/c1-8-7-10(8)4-2-3-9-5-6-9/h8-10H,2-7H2,1H3/t8-,10-/m1/s1 |
| InchiKey:            | GBESKWVEEIKQFO-PSASIEDQSA-N                                              |
| Formula:             | C10H18                                                                   |
| SMILES:              | CC1CC1CCCC1CC1                                                           |
| Mol. weight [g/mol]: | 138.25                                                                   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 147.11  | kJ/mol  | Joback Method  |
| hf            | -124.47 | kJ/mol  | Joback Method  |
| hfus          | 19.00   | kJ/mol  | Joback Method  |
| hvap          | 37.37   | kJ/mol  | Joback Method  |
| log10ws       | -3.07   |         | Crippen Method |
| logp          | 3.223   |         | Crippen Method |
| mcvol         | 130.040 | ml/mol  | McGowan Method |
| pc            | 2627.15 | kPa     | Joback Method  |
| rinpol        | 981.20  |         | NIST Webbook   |
| rinpol        | 981.20  |         | NIST Webbook   |
| rinpol        | 983.40  |         | NIST Webbook   |
| tb            | 437.01  | K       | Joback Method  |
| tc            | 626.35  | K       | Joback Method  |
| tf            | 234.10  | K       | Joback Method  |
| vc            | 0.508   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 286.74 | J/mol×K | 437.01          | Joback Method |
| cpg           | 305.06 | J/mol×K | 468.57          | Joback Method |
| cpg           | 322.35 | J/mol×K | 500.12          | Joback Method |
| cpg           | 338.68 | J/mol×K | 531.68          | Joback Method |
| cpg           | 354.08 | J/mol×K | 563.23          | Joback Method |
| cpg           | 368.62 | J/mol×K | 594.79          | Joback Method |
| cpg           | 382.35 | J/mol×K | 626.35          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0006447 | Pa×s | 234.10 | Joback Method |
| dvisc | 0.0006543 | Pa×s | 267.92 | Joback Method |
| dvisc | 0.0006618 | Pa×s | 301.74 | Joback Method |
| dvisc | 0.0006679 | Pa×s | 335.56 | Joback Method |
| dvisc | 0.0006729 | Pa×s | 369.37 | Joback Method |
| dvisc | 0.0006771 | Pa×s | 403.19 | Joback Method |
| dvisc | 0.0006807 | Pa×s | 437.01 | 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>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=R138151&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R138151&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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