

# Cyclohexane, 1,4-diethyl

Inchi:

InChI=1S/C10H20/c1-3-9-5-7-10(4-2)8-6-9/h9-10H,3-8H2,1-2H3

InchiKey:

SMAKEJNOUFLEEEJ-UHFFFAOYSA-N

Formula:

C10H20

SMILES:

CCC1CCC(CC)CC1

Mol. weight [g/mol]:

140.27

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 50.06   | kJ/mol  | Joback Method  |
| hf            | -215.75 | kJ/mol  | Joback Method  |
| hfus          | 14.56   | kJ/mol  | Joback Method  |
| hvap          | 37.97   | kJ/mol  | Joback Method  |
| log10ws       | -3.42   |         | Crippen Method |
| logp          | 3.613   |         | Crippen Method |
| mcvol         | 140.900 | ml/mol  | McGowan Method |
| pc            | 2485.07 | kPa     | Joback Method  |
| rinpol        | 1032.00 |         | NIST Webbook   |
| rinpol        | 1105.00 |         | NIST Webbook   |
| rinpol        | 1072.00 |         | NIST Webbook   |
| rinpol        | 1072.00 |         | NIST Webbook   |
| rinpol        | 1060.00 |         | NIST Webbook   |
| tb            | 443.08  | K       | Joback Method  |
| tc            | 639.52  | K       | Joback Method  |
| tf            | 205.60  | K       | Joback Method  |
| vc            | 0.527   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 299.73 | J/mol×K | 443.08          | Joback Method |
| cpg           | 319.51 | J/mol×K | 475.82          | Joback Method |
| cpg           | 338.41 | J/mol×K | 508.56          | Joback Method |
| cpg           | 356.42 | J/mol×K | 541.30          | Joback Method |
| cpg           | 373.57 | J/mol×K | 574.04          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 389.89    | J/mol×K | 606.78 | Joback Method |
| cpg   | 405.38    | J/mol×K | 639.52 | Joback Method |
| dvisc | 0.0050164 | Pa×s    | 205.60 | Joback Method |
| dvisc | 0.0020679 | Pa×s    | 245.18 | Joback Method |
| dvisc | 0.0010906 | Pa×s    | 284.76 | Joback Method |
| dvisc | 0.0006724 | Pa×s    | 324.34 | Joback Method |
| dvisc | 0.0004605 | Pa×s    | 363.92 | Joback Method |
| dvisc | 0.0003397 | Pa×s    | 403.50 | Joback Method |
| dvisc | 0.0002646 | Pa×s    | 443.08 | Joback Method |

## Sources

|                        |                                                                                                                                     |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------|
| <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=R443&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R443&amp;Units=SI</a> |
| <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>                   |

## 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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