

# Hexane, 1,6-dimethoxy-

|                      |                                                     |
|----------------------|-----------------------------------------------------|
| Other names:         | 1,6-Dimethoxyhexane                                 |
| Inchi:               | InChI=1S/C8H18O2/c1-9-7-5-3-4-6-8-10-2/h3-8H2,1-2H3 |
| InchiKey:            | GZHQUHIMIVEQFV-UHFFFAOYSA-N                         |
| Formula:             | C8H18O2                                             |
| SMILES:              | COCCCCCOC                                           |
| Mol. weight [g/mol]: | 146.23                                              |
| CAS:                 | 13179-98-1                                          |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -193.52 | kJ/mol  | Joback Method  |
| hf            | -472.89 | kJ/mol  | Joback Method  |
| hfus          | 18.85   | kJ/mol  | Joback Method  |
| hvap          | 38.22   | kJ/mol  | Joback Method  |
| log10ws       | -1.35   |         | Crippen Method |
| logp          | 1.840   |         | Crippen Method |
| mcvol         | 135.320 | ml/mol  | McGowan Method |
| pc            | 2450.74 | kPa     | Joback Method  |
| tb            | 427.28  | K       | Joback Method  |
| tc            | 591.50  | K       | Joback Method  |
| tf            | 224.38  | K       | Joback Method  |
| vc            | 0.519   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 282.41    | J/mol×K | 427.28          | Joback Method |
| cpg           | 341.34    | J/mol×K | 564.13          | Joback Method |
| cpg           | 330.24    | J/mol×K | 536.76          | Joback Method |
| cpg           | 318.79    | J/mol×K | 509.39          | Joback Method |
| cpg           | 307.00    | J/mol×K | 482.02          | Joback Method |
| cpg           | 294.87    | J/mol×K | 454.65          | Joback Method |
| cpg           | 352.10    | J/mol×K | 591.50          | Joback Method |
| dvisc         | 0.0001917 | Pa×s    | 427.28          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0002493 | Pa×s | 393.46 | Joback Method |
| dvisc | 0.0003408 | Pa×s | 359.65 | Joback Method |
| dvisc | 0.0004971 | Pa×s | 325.83 | Joback Method |
| dvisc | 0.0007912 | Pa×s | 292.01 | Joback Method |
| dvisc | 0.0014226 | Pa×s | 258.20 | Joback Method |
| dvisc | 0.0030523 | Pa×s | 224.38 | 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=C13179981&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13179981&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>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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