

# Methyl hexadecyl ether

|                      |                                                                              |
|----------------------|------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C17H36O/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-2/h3-17H2,1-2H3 |
| InchiKey:            | YOTHBMSACCHRLC-UHFFFAOYSA-N                                                  |
| Formula:             | C17H36O                                                                      |
| SMILES:              | CCCCCCCCCCCCCCCCOC                                                           |
| Mol. weight [g/mol]: | 256.47                                                                       |
| CAS:                 | 7307-53-1                                                                    |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -12.74  | kJ/mol  | Joback Method  |
| hf            | -526.43 | kJ/mol  | Joback Method  |
| hfus          | 40.97   | kJ/mol  | Joback Method  |
| hvap          | 55.85   | kJ/mol  | Joback Method  |
| log10ws       | -6.03   |         | Crippen Method |
| logp          | 6.114   |         | Crippen Method |
| mcvol         | 256.260 | ml/mol  | McGowan Method |
| pc            | 1216.59 | kPa     | Joback Method  |
| tb            | 610.78  | K       | Joback Method  |
| tc            | 770.13  | K       | Joback Method  |
| tf            | 303.58  | K       | Joback Method  |
| vc            | 1.006   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 699.43    | J/mol×K | 610.78          | Joback Method |
| cpg           | 788.91    | J/mol×K | 743.57          | Joback Method |
| cpg           | 772.45    | J/mol×K | 717.01          | Joback Method |
| cpg           | 755.28    | J/mol×K | 690.45          | Joback Method |
| cpg           | 737.40    | J/mol×K | 663.90          | Joback Method |
| cpg           | 718.79    | J/mol×K | 637.34          | Joback Method |
| cpg           | 804.69    | J/mol×K | 770.13          | Joback Method |
| dvisc         | 0.0001078 | Pa×s    | 610.78          | Joback Method |
| dvisc         | 0.0001462 | Pa×s    | 559.58          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0002108 | Pa×s | 508.38 | Joback Method |
| dvisc | 0.0003299 | Pa×s | 457.18 | Joback Method |
| dvisc | 0.0005781 | Pa×s | 405.98 | Joback Method |
| dvisc | 0.0011910 | Pa×s | 354.78 | Joback Method |
| dvisc | 0.0031310 | Pa×s | 303.58 | 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=C7307531&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7307531&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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