

# Hexadecyl propyl ether

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C19H40O/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-19-20-18-4-2/h3-19H2,1-2H |
| <b>InchiKey:</b>            | OU DWNTLJRZDXFC-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C19H40O   |
| <b>SMILES:</b>              | CCCCCCCCCCCCCCCCOCCC  |
| <b>Mol. weight [g/mol]:</b> | 284.52  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 4.10    | kJ/mol               | Joback Method  |
| hf            | -567.71 | kJ/mol               | Joback Method  |
| hfus          | 46.15   | kJ/mol               | Joback Method  |
| hvap          | 60.30   | kJ/mol               | Joback Method  |
| log10ws       | -6.86   |                      | Crippen Method |
| logp          | 6.894   |                      | Crippen Method |
| mvol          | 284.440 | ml/mol               | McGowan Method |
| pc            | 1068.66 | kPa                  | Joback Method  |
| rinpol        | 1980.00 |                      | NIST Webbook   |
| rinpol        | 1980.00 |                      | NIST Webbook   |
| tb            | 656.54  | K                    | Joback Method  |
| tc            | 817.30  | K                    | Joback Method  |
| tf            | 326.12  | K                    | Joback Method  |
| vc            | 1.117   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 815.08    | J/molxK | 656.54          | Joback Method |
| cpg           | 908.48    | J/molxK | 790.51          | Joback Method |
| cpg           | 891.37    | J/molxK | 763.71          | Joback Method |
| cpg           | 873.49    | J/molxK | 736.92          | Joback Method |
| cpg           | 854.83    | J/molxK | 710.13          | Joback Method |
| cpg           | 835.37    | J/molxK | 683.33          | Joback Method |
| cpg           | 924.85    | J/molxK | 817.30          | Joback Method |
| dvisc         | 0.0000849 | Paxs    | 656.54          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001157 | Paxs | 601.47 | Joback Method |
| dvisc | 0.0001679 | Paxs | 546.40 | Joback Method |
| dvisc | 0.0002648 | Paxs | 491.33 | Joback Method |
| dvisc | 0.0004686 | Paxs | 436.26 | Joback Method |
| dvisc | 0.0009778 | Paxs | 381.19 | Joback Method |
| dvisc | 0.0026162 | Paxs | 326.12 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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=U406279&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406279&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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