

# Hexacosyl methyl ether

|                             |                                                                                   |
|-----------------------------|-----------------------------------------------------------------------------------|
| <b>Inchi:</b>               | InChI=1S/C27H56O/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25 |
| <b>InchiKey:</b>            | NPHUNKXXXLITDL-UHFFFAOYSA-N                                                       |
| <b>Formula:</b>             | C27H56O                                                                           |
| <b>SMILES:</b>              | CCCCCCCCCCCCCCCCCCCCCCCCCCCCOC                                                    |
| <b>Mol. weight [g/mol]:</b> | 396.73                                                                            |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 71.46   | kJ/mol  | Joback Method  |
| hf            | -732.83 | kJ/mol  | Joback Method  |
| hfus          | 66.87   | kJ/mol  | Joback Method  |
| hvap          | 78.11   | kJ/mol  | Joback Method  |
| log10ws       | -10.21  |         | Crippen Method |
| logp          | 10.015  |         | Crippen Method |
| mcvol         | 397.160 | ml/mol  | McGowan Method |
| pc            | 682.78  | kPa     | Joback Method  |
| rinpol        | 2838.00 |         | NIST Webbook   |
| tb            | 839.58  | K       | Joback Method  |
| tc            | 1029.43 | K       | Joback Method  |
| tf            | 416.28  | K       | Joback Method  |
| vc            | 1.565   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1318.29   | J/mol×K | 839.58          | Joback Method |
| cpg           | 1343.10   | J/mol×K | 871.22          | Joback Method |
| cpg           | 1366.56   | J/mol×K | 902.86          | Joback Method |
| cpg           | 1388.75   | J/mol×K | 934.50          | Joback Method |
| cpg           | 1409.69   | J/mol×K | 966.14          | Joback Method |
| cpg           | 1429.45   | J/mol×K | 997.78          | Joback Method |
| cpg           | 1448.06   | J/mol×K | 1029.43         | Joback Method |
| dvisc         | 0.0010370 | Pa×s    | 416.28          | Joback Method |
| dvisc         | 0.0003681 | Pa×s    | 486.83          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001699 | Pa×s | 557.38 | Joback Method |
| dvisc | 0.0000933 | Pa×s | 627.93 | Joback Method |
| dvisc | 0.0000578 | Pa×s | 698.48 | Joback Method |
| dvisc | 0.0000391 | Pa×s | 769.03 | Joback Method |
| dvisc | 0.0000282 | Pa×s | 839.58 | 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=U406297&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406297&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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