

# Benzene, 1,3-dimethoxy-4-nonyl

|                      |                                                                                   |
|----------------------|-----------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C17H28O2/c1-4-5-6-7-8-9-10-11-15-12-13-16(18-2)14-17(15)19-3/h12-14H,4-1 |
| InchiKey:            | KDNSWIKIDFIPCS-UHFFFAOYSA-N                                                       |
| Formula:             | C17H28O2                                                                          |
| SMILES:              | CCCCCCCCCc1ccc(OC)cc1OC                                                           |
| Mol. weight [g/mol]: | 264.40                                                                            |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -24.59  | kJ/mol  | Joback Method  |
| hf            | -445.06 | kJ/mol  | Joback Method  |
| hfus          | 35.42   | kJ/mol  | Joback Method  |
| hvap          | 61.86   | kJ/mol  | Joback Method  |
| log10ws       | -5.44   |         | Crippen Method |
| logp          | 4.997   |         | Crippen Method |
| mcvol         | 238.370 | ml/mol  | McGowan Method |
| pc            | 1498.83 | kPa     | Joback Method  |
| rinpol        | 1982.00 |         | NIST Webbook   |
| rinpol        | 1982.00 |         | NIST Webbook   |
| tb            | 669.84  | K       | Joback Method  |
| tc            | 857.12  | K       | Joback Method  |
| tf            | 377.27  | K       | Joback Method  |
| vc            | 0.915   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 658.97    | J/mol×K | 669.84          | Joback Method |
| cpg           | 677.24    | J/mol×K | 701.05          | Joback Method |
| cpg           | 694.63    | J/mol×K | 732.27          | Joback Method |
| cpg           | 711.13    | J/mol×K | 763.48          | Joback Method |
| cpg           | 726.77    | J/mol×K | 794.69          | Joback Method |
| cpg           | 741.55    | J/mol×K | 825.91          | Joback Method |
| cpg           | 755.49    | J/mol×K | 857.12          | Joback Method |
| dvisc         | 0.0009250 | Pa×s    | 377.27          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0004912 | Pa×s | 426.03 | Joback Method |
| dvisc | 0.0002971 | Pa×s | 474.79 | Joback Method |
| dvisc | 0.0001973 | Pa×s | 523.56 | Joback Method |
| dvisc | 0.0001405 | Pa×s | 572.32 | Joback Method |
| dvisc | 0.0001055 | Pa×s | 621.08 | Joback Method |
| dvisc | 0.0000826 | Pa×s | 669.84 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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=R143089&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R143089&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>                                 |

## 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>mccvol:</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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