

# 2-Octanol, 8,8-dimethoxy-

|                      |                                                                     |
|----------------------|---------------------------------------------------------------------|
| Inchi:               | InChI=1S/C10H22O3/c1-9(11)7-5-4-6-8-10(12-2)13-3/h9-11H,4-8H2,1-3H3 |
| InchiKey:            | SGFZPZDYTTDDIOQ-UHFFFAOYSA-N                                        |
| Formula:             | C10H22O3                                                            |
| SMILES:              | COC(CCCCCC(C)O)OC                                                   |
| Mol. weight [g/mol]: | 190.28                                                              |
| CAS:                 | 312305-55-8                                                         |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -318.38 | kJ/mol  | Joback Method  |
| hf            | -676.96 | kJ/mol  | Joback Method  |
| hfus          | 21.07   | kJ/mol  | Joback Method  |
| hvap          | 58.58   | kJ/mol  | Joback Method  |
| log10ws       | -2.17   |         | Crippen Method |
| logp          | 1.937   |         | Crippen Method |
| mcvol         | 169.370 | ml/mol  | McGowan Method |
| pc            | 2258.96 | kPa     | Joback Method  |
| tb            | 564.34  | K       | Joback Method  |
| tc            | 728.46  | K       | Joback Method  |
| tf            | 277.74  | K       | Joback Method  |
| vc            | 0.638   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 434.11    | J/mol×K | 564.34          | Joback Method |
| cpg           | 447.59    | J/mol×K | 591.69          | Joback Method |
| cpg           | 460.60    | J/mol×K | 619.05          | Joback Method |
| cpg           | 473.12    | J/mol×K | 646.40          | Joback Method |
| cpg           | 485.16    | J/mol×K | 673.76          | Joback Method |
| cpg           | 496.72    | J/mol×K | 701.11          | Joback Method |
| cpg           | 507.80    | J/mol×K | 728.46          | Joback Method |
| dvisc         | 0.0244859 | Pa×s    | 277.74          | Joback Method |
| dvisc         | 0.0043018 | Pa×s    | 325.51          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0011795 | Pa×s | 373.27 | Joback Method |
| dvisc | 0.0004337 | Pa×s | 421.04 | Joback Method |
| dvisc | 0.0001956 | Pa×s | 468.81 | Joback Method |
| dvisc | 0.0001022 | Pa×s | 516.57 | Joback Method |
| dvisc | 0.0000596 | Pa×s | 564.34 | 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=C312305558&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C312305558&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>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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