

# 2,3-diethoxy-1-propanol

|                      |                                                          |
|----------------------|----------------------------------------------------------|
| Inchi:               | InChI=1S/C7H16O3/c1-3-9-6-7(5-8)10-4-2/h7-8H,3-6H2,1-2H3 |
| InchiKey:            | CCLNWKPQPZBSEI-UHFFFAOYSA-N                              |
| Formula:             | C7H16O3                                                  |
| SMILES:              | CCOCC(CO)OCC                                             |
| Mol. weight [g/mol]: | 148.20                                                   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -341.20 | kJ/mol  | Joback Method  |
| hf            | -609.76 | kJ/mol  | Joback Method  |
| hfus          | 16.83   | kJ/mol  | Joback Method  |
| hvap          | 52.29   | kJ/mol  | Joback Method  |
| log10ws       | -0.30   |         | Crippen Method |
| logp          | 0.420   |         | Crippen Method |
| mcvol         | 127.100 | ml/mol  | McGowan Method |
| pc            | 3005.73 | kPa     | Joback Method  |
| ripol         | 1520.00 |         | NIST Webbook   |
| tb            | 496.14  | K       | Joback Method  |
| tc            | 659.77  | K       | Joback Method  |
| tf            | 258.93  | K       | Joback Method  |
| vc            | 0.476   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 295.11    | J/mol×K | 496.14          | Joback Method |
| cpg           | 305.70    | J/mol×K | 523.41          | Joback Method |
| cpg           | 315.98    | J/mol×K | 550.68          | Joback Method |
| cpg           | 325.94    | J/mol×K | 577.96          | Joback Method |
| cpg           | 335.57    | J/mol×K | 605.23          | Joback Method |
| cpg           | 344.88    | J/mol×K | 632.50          | Joback Method |
| cpg           | 353.86    | J/mol×K | 659.77          | Joback Method |
| dvisc         | 0.0271956 | Pa×s    | 258.93          | Joback Method |
| dvisc         | 0.0059483 | Pa×s    | 298.47          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0018565 | Pa×s | 338.00 | Joback Method |
| dvisc | 0.0007395 | Pa×s | 377.53 | Joback Method |
| dvisc | 0.0003507 | Pa×s | 417.07 | Joback Method |
| dvisc | 0.0001893 | Pa×s | 456.61 | Joback Method |
| dvisc | 0.0001127 | Pa×s | 496.14 | 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=R330337&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R330337&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>ripol:</b>   | 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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