

# Ethanol, 2,2'-oxybis-, diacetate

|                      |                                                                                                                                                                                   |
|----------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | Diethylene glycol, diacetate<br>Oxydiethylene acetate<br>Diglycol, diacetate<br>dioxyethylene glycol diacetate<br>2-(2-Acetyloxyethoxy)ethyl acetate<br>oxydiethylene di(acetate) |
| Inchi:               | InChI=1S/C8H14O5/c1-7(9)12-5-3-11-4-6-13-8(2)10/h3-6H2,1-2H3                                                                                                                      |
| InchiKey:            | UBPGILLNMDGSDS-UHFFFAOYSA-N                                                                                                                                                       |
| Formula:             | C8H14O5                                                                                                                                                                           |
| SMILES:              | CC(=O)OCCOCCOC(C)=O                                                                                                                                                               |
| Mol. weight [g/mol]: | 190.19                                                                                                                                                                            |
| CAS:                 | 628-68-2                                                                                                                                                                          |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| gf            | -556.36 | kJ/mol | Joback Method  |
| hf            | -830.27 | kJ/mol | Joback Method  |
| hfus          | 23.24   | kJ/mol | Joback Method  |
| hvap          | 54.12   | kJ/mol | Joback Method  |
| log10ws       | 0.02    |        | Crippen Method |
| logp          | 0.129   |        | Crippen Method |
| mcvol         | 144.330 | ml/mol | McGowan Method |
| pc            | 2738.28 | kPa    | Joback Method  |
| rinpol        | 1278.00 |        | NIST Webbook   |
| rinpol        | 1285.00 |        | NIST Webbook   |
| rinpol        | 1278.00 |        | NIST Webbook   |
| rinpol        | 1282.00 |        | NIST Webbook   |
| rinpol        | 1278.00 |        | NIST Webbook   |
| rinpol        | 1283.00 |        | NIST Webbook   |
| rinpol        | 1303.00 |        | NIST Webbook   |
| rinpol        | 1280.00 |        | NIST Webbook   |
| rinpol        | 1282.60 |        | NIST Webbook   |
| rinpol        | 1282.00 |        | NIST Webbook   |
| rinpol        | 1281.00 |        | NIST Webbook   |
| rinpol        | 1279.00 |        | NIST Webbook   |
| rinpol        | 1281.00 |        | NIST Webbook   |
| rinpol        | 1280.00 |        | NIST Webbook   |

|       |         |                      |               |
|-------|---------|----------------------|---------------|
| ripol | 1970.00 |                      | NIST Webbook  |
| ripol | 1937.00 |                      | NIST Webbook  |
| ripol | 1970.00 |                      | NIST Webbook  |
| tb    | 557.44  | K                    | Joback Method |
| tc    | 740.14  | K                    | Joback Method |
| tf    | 346.47  | K                    | Joback Method |
| vc    | 0.549   | m <sup>3</sup> /kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 345.92    | J/mol×K | 557.44          | Joback Method |
| cpg           | 357.32    | J/mol×K | 587.89          | Joback Method |
| cpg           | 368.32    | J/mol×K | 618.34          | Joback Method |
| cpg           | 378.91    | J/mol×K | 648.79          | Joback Method |
| cpg           | 389.07    | J/mol×K | 679.24          | Joback Method |
| cpg           | 398.77    | J/mol×K | 709.69          | Joback Method |
| cpg           | 408.02    | J/mol×K | 740.14          | Joback Method |
| dvisc         | 0.0015072 | Pa×s    | 346.47          | Joback Method |
| dvisc         | 0.0009040 | Pa×s    | 381.63          | Joback Method |
| dvisc         | 0.0005910 | Pa×s    | 416.79          | Joback Method |
| dvisc         | 0.0004128 | Pa×s    | 451.96          | Joback Method |
| dvisc         | 0.0003037 | Pa×s    | 487.12          | Joback Method |
| dvisc         | 0.0002328 | Pa×s    | 522.28          | Joback Method |
| dvisc         | 0.0001846 | Pa×s    | 557.44          | Joback Method |

## Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 395.70 | K    | 2.10           | NIST Webbook |

## Sources

Joback Method:

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C628682&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

## 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>hvac:</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>ripol:</b>   | Polar retention indices                         |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tbrp:</b>    | Boiling point at reduced pressure               |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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