

# Tetraethylene glycol, pentyl ether, acetate

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | 2-(2-(2-Pentoxy-ethoxy)-ethoxy)-ethoxy)-ethyl acetate                            |
| <b>Inchi:</b>               | InChI=1S/C15H30O6/c1-3-4-5-6-17-7-8-18-9-10-19-11-12-20-13-14-21-15(2)16/h3-14H2 |
| <b>InchiKey:</b>            | DFTAUBRZUHAJGX-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C15H30O6   |
| <b>SMILES:</b>              | CCCCCOCCOCCOCCOCCOC(C)=O   |
| <b>Mol. weight [g/mol]:</b> | 306.40   |

## Physical Properties

| Property code | Value    | Unit                 | Source         |
|---------------|----------|----------------------|----------------|
| gf            | -578.50  | kJ/mol               | Joback Method  |
| hf            | -1126.61 | kJ/mol               | Joback Method  |
| hfus          | 42.14    | kJ/mol               | Joback Method  |
| hvap          | 67.78    | kJ/mol               | Joback Method  |
| log10ws       | -1.31    |                      | Crippen Method |
| logp          | 1.806    |                      | Crippen Method |
| mcvol         | 253.130  | ml/mol               | McGowan Method |
| pc            | 1392.29  | kPa                  | Joback Method  |
| rinpol        | 2073.00  |                      | NIST Webbook   |
| tb            | 708.57   | K                    | Joback Method  |
| tc            | 879.47   | K                    | Joback Method  |
| tf            | 419.89   | K                    | Joback Method  |
| vc            | 0.972    | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 741.92    | J/molxK | 708.57          | Joback Method |
| cpg           | 817.74    | J/molxK | 850.99          | Joback Method |
| cpg           | 804.18    | J/molxK | 822.51          | Joback Method |
| cpg           | 789.80    | J/molxK | 794.02          | Joback Method |
| cpg           | 774.62    | J/molxK | 765.54          | Joback Method |
| cpg           | 758.66    | J/molxK | 737.05          | Joback Method |
| cpg           | 830.46    | J/molxK | 879.47          | Joback Method |
| dvisc         | 0.0000481 | Paxs    | 708.57          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0000627 | Paxs | 660.46 | Joback Method |
| dvisc | 0.0000852 | Paxs | 612.34 | Joback Method |
| dvisc | 0.0001220 | Paxs | 564.23 | Joback Method |
| dvisc | 0.0001868 | Paxs | 516.12 | Joback Method |
| dvisc | 0.0003123 | Paxs | 468.00 | Joback Method |
| dvisc | 0.0005874 | Paxs | 419.89 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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=R188626&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R188626&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>                                     |

## 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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