

# 2-Hydroxyethyl pentanoate

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C7H14O3/c1-2-3-4-7(9)10-6-5-8/h8H,2-6H2,1H3 |
| <b>InchiKey:</b>            | GFNKWCJODVREDZ-UHFFFAOYSA-N                          |
| <b>Formula:</b>             | C7H14O3  |
| <b>SMILES:</b>              | CCCCC(=O)OCCO  |
| <b>Mol. weight [g/mol]:</b> | 146.18   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -362.68 | kJ/mol               | Joback Method  |
| hf            | -584.84 | kJ/mol               | Joback Method  |
| hfus          | 20.76   | kJ/mol               | Joback Method  |
| hvap          | 57.01   | kJ/mol               | Joback Method  |
| log10ws       | -0.88   |                      | Crippen Method |
| logp          | 0.712   |                      | Crippen Method |
| mcvol         | 122.800 | ml/mol               | McGowan Method |
| pc            | 3257.86 | kPa                  | Joback Method  |
| rinsol        | 1096.00 |                      | NIST Webbook   |
| tb            | 528.03  | K                    | Joback Method  |
| tc            | 697.73  | K                    | Joback Method  |
| tf            | 301.63  | K                    | Joback Method  |
| vc            | 0.470   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 288.44    | J/molxK | 528.03          | Joback Method |
| cpg           | 298.28    | J/molxK | 556.31          | Joback Method |
| cpg           | 307.76    | J/molxK | 584.60          | Joback Method |
| cpg           | 316.88    | J/molxK | 612.88          | Joback Method |
| cpg           | 325.65    | J/molxK | 641.16          | Joback Method |
| cpg           | 334.05    | J/molxK | 669.45          | Joback Method |
| cpg           | 342.10    | J/molxK | 697.73          | Joback Method |
| dvisc         | 0.0101756 | Paxs    | 301.63          | Joback Method |
| dvisc         | 0.0032968 | Paxs    | 339.36          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0013384 | Paxs | 377.10 | Joback Method |
| dvisc | 0.0006402 | Paxs | 414.83 | Joback Method |
| dvisc | 0.0003463 | Paxs | 452.56 | Joback Method |
| dvisc | 0.0002059 | Paxs | 490.30 | Joback Method |
| dvisc | 0.0001318 | Paxs | 528.03 | 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=R540539&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R540539&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>                                 |
| <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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