

# Propane, 1,1,1-triethoxy-

|                      |                                                                                                                             |
|----------------------|-----------------------------------------------------------------------------------------------------------------------------|
| Other names:         | Orthopropionic acid, triethyl ester<br>Ethyl orthopropionate<br>Orthopropionic acid ethyl ester<br>Triethyl orthopropionate |
| Inchi:               | InChI=1S/C9H20O3/c1-5-9(10-6-2,11-7-3)12-8-4/h5-8H2,1-4H3                                                                   |
| InchiKey:            | FGWYWKIOMUZSQF-UHFFFAOYSA-N                                                                                                 |
| Formula:             | C9H20O3                                                                                                                     |
| SMILES:              | CCOC(CC)(OCC)OCC                                                                                                            |
| Mol. weight [g/mol]: | 176.25                                                                                                                      |
| CAS:                 | 115-80-0                                                                                                                    |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -287.26 | kJ/mol  | Joback Method  |
| hf            | -634.50 | kJ/mol  | Joback Method  |
| hfus          | 15.22   | kJ/mol  | Joback Method  |
| hvap          | 41.56   | kJ/mol  | Joback Method  |
| log10ws       | -1.95   |         | Crippen Method |
| logp          | 2.160   |         | Crippen Method |
| mcvol         | 155.280 | ml/mol  | McGowan Method |
| pc            | 2237.64 | kPa     | Joback Method  |
| tb            | 430.70  | K       | NIST Webbook   |
| tc            | 642.31  | K       | Joback Method  |
| tf            | 260.30  | K       | Joback Method  |
| vc            | 0.583   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 353.16 | J/mol×K | 469.35          | Joback Method |
| cpg           | 367.65 | J/mol×K | 498.18          | Joback Method |
| cpg           | 381.64 | J/mol×K | 527.00          | Joback Method |
| cpg           | 395.14 | J/mol×K | 555.83          | Joback Method |
| cpg           | 408.14 | J/mol×K | 584.66          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 420.65    | J/mol×K | 613.48 | Joback Method |
| cpg   | 432.66    | J/mol×K | 642.31 | Joback Method |
| dvisc | 0.0031085 | Pa×s    | 260.30 | Joback Method |
| dvisc | 0.0013963 | Pa×s    | 295.14 | Joback Method |
| dvisc | 0.0007427 | Pa×s    | 329.98 | Joback Method |
| dvisc | 0.0004457 | Pa×s    | 364.82 | Joback Method |
| dvisc | 0.0002923 | Pa×s    | 399.67 | Joback Method |
| dvisc | 0.0002052 | Pa×s    | 434.51 | Joback Method |
| dvisc | 0.0001518 | Pa×s    | 469.35 | Joback Method |

## Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 317.20 | K    | 1.00           | NIST Webbook |

## Sources

|                 |                                                                                                                                           |
|-----------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| Joback Method:  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C115800&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C115800&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>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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