

# 1,4-ANHYDRO-L-THREITOL

|                      |                                                                                             |
|----------------------|---------------------------------------------------------------------------------------------|
| Other names:         | 1,4-Anhydro-l-threitol<br>Tetrahydro-3,4-furandiol, trans<br>trans-tetrahydrofuran-3,4-diol |
| Inchi:               | InChI=1S/C4H8O3/c5-3-1-7-2-4(3)6/h3-6H,1-2H2                                                |
| InchiKey:            | SSYDTHANSGMJTP-UHFFFAOYSA-N                                                                 |
| Formula:             | C4H8O3                                                                                      |
| SMILES:              | OC1COCC1O                                                                                   |
| Mol. weight [g/mol]: | 104.10                                                                                      |

## Physical Properties

| Property code | Value  | Unit   | Source         |
|---------------|--------|--------|----------------|
| hfus          | 17.28  | kJ/mol | Joback Method  |
| logp          | -1.262 |        | Crippen Method |
| mcpvol        | 73.970 | ml/mol | McGowan Method |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 182.39    | J/mol×K | 512.84          | Joback Method |
| cpg           | 190.65    | J/mol×K | 543.13          | Joback Method |
| cpg           | 198.51    | J/mol×K | 573.42          | Joback Method |
| cpg           | 205.99    | J/mol×K | 603.71          | Joback Method |
| cpg           | 213.09    | J/mol×K | 634.00          | Joback Method |
| cpg           | 219.82    | J/mol×K | 664.29          | Joback Method |
| cpg           | 226.18    | J/mol×K | 694.58          | Joback Method |
| dvisc         | 0.0575968 | Pa×s    | 289.71          | Joback Method |
| dvisc         | 0.0118979 | Pa×s    | 326.90          | Joback Method |
| dvisc         | 0.0033920 | Pa×s    | 364.09          | Joback Method |
| dvisc         | 0.0012203 | Pa×s    | 401.27          | Joback Method |
| dvisc         | 0.0005221 | Pa×s    | 438.46          | Joback Method |
| dvisc         | 0.0002551 | Pa×s    | 475.65          | Joback Method |
| dvisc         | 0.0001383 | Pa×s    | 512.84          | Joback Method |

# Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 393.20 | K    | 2.10           | NIST Webbook |

## Sources

|                           |                                                                                                                                               |
|---------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| McGowan Method:           | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>                             |
| Cheméo Relay (1.0):       |                                                                                                                                               |
| Cheméo Relay (1.0, beta): |                                                                                                                                               |
| NIST Webbook:             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C22554741&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C22554741&amp;Units=SI</a> |
| Joback Method:            | <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>hfus:</b>  | Enthalpy of fusion at standard conditions |
| <b>logp:</b>  | Octanol/Water partition coefficient       |
| <b>mcvol:</b> | McGowan's characteristic volume           |
| <b>tbrp:</b>  | Boiling point at reduced pressure         |

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