

# Oxirane, propyl-

|                      |                                                                                                                                               |
|----------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | Pentane, 1,2-epoxy-<br>Pentene 1,2-oxide<br>Propylethylene oxide<br>Propyloxirane<br>1-Pentene oxide<br>1,2-Epoxy pentane<br>2-Propyl-oxirane |
| Inchi:               | InChI=1S/C5H10O/c1-2-3-5-4-6-5/h5H,2-4H2,1H3                                                                                                  |
| InchiKey:            | SYURNNNQIFDVCA-UHFFFAOYSA-N                                                                                                                   |
| Formula:             | C5H10O                                                                                                                                        |
| SMILES:              | CCCC1CO1                                                                                                                                      |
| Mol. weight [g/mol]: | 86.13                                                                                                                                         |
| CAS:                 | 1003-14-1                                                                                                                                     |

## Physical Properties

| Property code | Value         | Unit   | Source         |
|---------------|---------------|--------|----------------|
| gf            | -34.15        | kJ/mol | Joback Method  |
| hf            | -205.73       | kJ/mol | Joback Method  |
| hfus          | 14.82         | kJ/mol | Joback Method  |
| hvap          | 31.15         | kJ/mol | Joback Method  |
| log10ws       | -1.01         |        | Crippen Method |
| logp          | 1.185         |        | Crippen Method |
| mcpvol        | 76.320        | ml/mol | McGowan Method |
| pc            | 4021.02       | kPa    | Joback Method  |
| rinpol        | 624.90        |        | NIST Webbook   |
| rinpol        | 666.00        |        | NIST Webbook   |
| rinpol        | 624.00        |        | NIST Webbook   |
| rinpol        | 666.00        |        | NIST Webbook   |
| rinpol        | 624.90        |        | NIST Webbook   |
| rinpol        | 624.70        |        | NIST Webbook   |
| rinpol        | 624.50        |        | NIST Webbook   |
| rinpol        | 625.00        |        | NIST Webbook   |
| rinpol        | 625.00        |        | NIST Webbook   |
| rinpol        | 624.00        |        | NIST Webbook   |
| tb            | 364.85 ± 0.50 | K      | NIST Webbook   |
| tc            | 528.16        | K      | Joback Method  |
| tf            | 190.62        | K      | Joback Method  |

# Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 134.15    | J/mol×K | 347.49          | Joback Method |
| cpg           | 181.98    | J/mol×K | 498.05          | Joback Method |
| cpg           | 173.40    | J/mol×K | 467.94          | Joback Method |
| cpg           | 164.35    | J/mol×K | 437.83          | Joback Method |
| cpg           | 154.81    | J/mol×K | 407.71          | Joback Method |
| cpg           | 144.75    | J/mol×K | 377.60          | Joback Method |
| cpg           | 190.11    | J/mol×K | 528.16          | Joback Method |
| dvisc         | 0.0003539 | Pa×s    | 347.49          | Joback Method |
| dvisc         | 0.0003972 | Pa×s    | 321.35          | Joback Method |
| dvisc         | 0.0004549 | Pa×s    | 295.20          | Joback Method |
| dvisc         | 0.0005349 | Pa×s    | 269.06          | Joback Method |
| dvisc         | 0.0006513 | Pa×s    | 242.91          | Joback Method |
| dvisc         | 0.0008316 | Pa×s    | 216.77          | Joback Method |
| dvisc         | 0.0011356 | Pa×s    | 190.62          | Joback Method |

## Sources

|                 |                                                                                                                                             |
|-----------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1003141&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1003141&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>                           |
| 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>                       |

## 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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