

# Oxirane, 2-ethyl-3-methyl-, trans-

|                      |                                                             |
|----------------------|-------------------------------------------------------------|
| Other names:         | 2-Ethyl-3-methyl-oxirane (E)                                |
| Inchi:               | InChI=1S/C5H10O/c1-3-5-4(2)6-5/h4-5H,3H2,1-2H3/t4-,5-/m0/s1 |
| InchiKey:            | BCJPEZMFAKOJPM-WHFBIAKZSA-N                                 |
| Formula:             | C5H10O                                                      |
| SMILES:              | CCC1OC1C                                                    |
| Mol. weight [g/mol]: | 86.13                                                       |
| CAS:                 | 3203-98-3                                                   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -41.86  | kJ/mol  | Joback Method  |
| hf            | -226.07 | kJ/mol  | Joback Method  |
| hfus          | 15.89   | kJ/mol  | Joback Method  |
| hvap          | 30.84   | kJ/mol  | Joback Method  |
| log10ws       | -1.12   |         | Crippen Method |
| logp          | 1.184   |         | Crippen Method |
| mcvol         | 76.320  | ml/mol  | McGowan Method |
| pc            | 3857.88 | kPa     | Joback Method  |
| rinpol        | 652.00  |         | NIST Webbook   |
| rinpol        | 654.90  |         | NIST Webbook   |
| rinpol        | 655.00  |         | NIST Webbook   |
| rinpol        | 655.00  |         | NIST Webbook   |
| rinpol        | 655.00  |         | NIST Webbook   |
| rinpol        | 655.00  |         | NIST Webbook   |
| rinpol        | 655.10  |         | NIST Webbook   |
| tb            | 342.82  | K       | Joback Method  |
| tc            | 522.72  | K       | Joback Method  |
| tf            | 186.38  | K       | Joback Method  |
| vc            | 0.292   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 134.69 | J/mol×K | 342.82          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 145.40    | J/mol×K | 372.80 | Joback Method |
| cpg   | 155.61    | J/mol×K | 402.79 | Joback Method |
| cpg   | 165.35    | J/mol×K | 432.77 | Joback Method |
| cpg   | 174.63    | J/mol×K | 462.75 | Joback Method |
| cpg   | 183.47    | J/mol×K | 492.73 | Joback Method |
| cpg   | 191.88    | J/mol×K | 522.72 | Joback Method |
| dvisc | 0.0005411 | Pa×s    | 186.38 | Joback Method |
| dvisc | 0.0004606 | Pa×s    | 212.45 | Joback Method |
| dvisc | 0.0004062 | Pa×s    | 238.53 | Joback Method |
| dvisc | 0.0003671 | Pa×s    | 264.60 | Joback Method |
| dvisc | 0.0003379 | Pa×s    | 290.67 | Joback Method |
| dvisc | 0.0003153 | Pa×s    | 316.75 | Joback Method |
| dvisc | 0.0002973 | Pa×s    | 342.82 | Joback Method |

## Sources

|                        |                                                                                                                                             |
|------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| <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>                                       |
| <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=C3203983&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3203983&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>                                   |

## 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                   |

**vc:** Critical Volume

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