

# 1-Propene, 1,1'-oxybis-, (Z,Z)-

|                      |                                                       |
|----------------------|-------------------------------------------------------|
| Other names:         | Propenyl ether, (Z,Z)-<br>cis, cis-Dipropenyl ether   |
| Inchi:               | InChI=1S/C6H10O/c1-3-5-7-6-4-2/h3-6H,1-2H3/b5-3-,6-4- |
| InchiKey:            | ZKJNETINGMOHJG-GLIMQPGKSA-N                           |
| Formula:             | C6H10O                                                |
| SMILES:              | CC=COC=CC                                             |
| Mol. weight [g/mol]: | 98.14                                                 |
| CAS:                 | 4696-27-9                                             |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 55.08   | kJ/mol  | Joback Method  |
| hf            | -64.95  | kJ/mol  | Joback Method  |
| hfus          | 12.89   | kJ/mol  | Joback Method  |
| hvap          | 31.28   | kJ/mol  | Joback Method  |
| log10ws       | -2.12   |         | Crippen Method |
| logp          | 2.070   |         | Crippen Method |
| mcvol         | 92.670  | ml/mol  | McGowan Method |
| pc            | 3431.89 | kPa     | Joback Method  |
| tb            | 367.42  | K       | Joback Method  |
| tc            | 550.12  | K       | Joback Method  |
| tf            | 169.45  | K       | Joback Method  |
| vc            | 0.349   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 153.37 | J/mol×K | 367.42          | Joback Method |
| cpg           | 163.10 | J/mol×K | 397.87          | Joback Method |
| cpg           | 172.40 | J/mol×K | 428.32          | Joback Method |
| cpg           | 181.26 | J/mol×K | 458.77          | Joback Method |
| cpg           | 189.72 | J/mol×K | 489.22          | Joback Method |
| cpg           | 197.78 | J/mol×K | 519.67          | Joback Method |
| cpg           | 205.46 | J/mol×K | 550.12          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0030234 | Pa×s | 169.45 | Joback Method |
| dvisc | 0.0012125 | Pa×s | 202.44 | Joback Method |
| dvisc | 0.0006282 | Pa×s | 235.44 | Joback Method |
| dvisc | 0.0003826 | Pa×s | 268.44 | Joback Method |
| dvisc | 0.0002597 | Pa×s | 301.43 | Joback Method |
| dvisc | 0.0001903 | Pa×s | 334.43 | Joback Method |
| dvisc | 0.0001474 | Pa×s | 367.42 | 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=C4696279&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4696279&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>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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