

# Benzene, 1,1'-[1,2-ethanediylbis(oxy)]bis-

|                      |                                                                                                                |
|----------------------|----------------------------------------------------------------------------------------------------------------|
| Other names:         | Ethane, 1,2-diphenoxy-<br>Ethylene glycol diphenyl ether<br>1,2-Diphenoxyethane<br>2-Phenoxyethyl phenyl ether |
| Inchi:               | InChI=1S/C14H14O2/c1-3-7-13(8-4-1)15-11-12-16-14-9-5-2-6-10-14/h1-10H,11-12H2                                  |
| InchiKey:            | XCSGHNKDXGYELG-UHFFFAOYSA-N                                                                                    |
| Formula:             | C14H14O2                                                                                                       |
| SMILES:              | c1ccc(OCCOc2ccccc2)cc1                                                                                         |
| Mol. weight [g/mol]: | 214.26                                                                                                         |
| CAS:                 | 104-66-5                                                                                                       |

## Physical Properties

| Property code | Value       | Unit    | Source         |
|---------------|-------------|---------|----------------|
| gf            | 81.82       | kJ/mol  | Joback Method  |
| hf            | -123.67     | kJ/mol  | Joback Method  |
| hfus          | 22.47       | kJ/mol  | Joback Method  |
| hvap          | 56.13       | kJ/mol  | Joback Method  |
| ie            | 8.39 ± 0.05 | eV      | NIST Webbook   |
| log10ws       | -3.36       |         | Crippen Method |
| logp          | 3.144       |         | Crippen Method |
| mcvol         | 172.340     | ml/mol  | McGowan Method |
| pc            | 2673.54     | kPa     | Joback Method  |
| rinpol        | 1810.60     |         | NIST Webbook   |
| tb            | 617.92      | K       | Joback Method  |
| tc            | 850.54      | K       | Joback Method  |
| tf            | 344.84      | K       | Joback Method  |
| vc            | 0.639       | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 423.99 | J/mol×K | 617.92          | Joback Method |
| cpg           | 496.15 | J/mol×K | 811.77          | Joback Method |
| cpg           | 483.91 | J/mol×K | 773.00          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 470.61    | J/mol×K | 734.23 | Joback Method |
| cpg   | 456.21    | J/mol×K | 695.46 | Joback Method |
| cpg   | 440.68    | J/mol×K | 656.69 | Joback Method |
| cpg   | 507.36    | J/mol×K | 850.54 | Joback Method |
| dvisc | 0.0001160 | Pa×s    | 617.92 | Joback Method |
| dvisc | 0.0001489 | Pa×s    | 572.41 | Joback Method |
| dvisc | 0.0001996 | Pa×s    | 526.89 | Joback Method |
| dvisc | 0.0002826 | Pa×s    | 481.38 | Joback Method |
| dvisc | 0.0004305 | Pa×s    | 435.87 | Joback Method |
| dvisc | 0.0007233 | Pa×s    | 390.35 | Joback Method |
| dvisc | 0.0013936 | Pa×s    | 344.84 | Joback Method |

## Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 455.70 | K    | 1.60           | NIST Webbook |

## Sources

|                 |                                                                                                                                           |
|-----------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C104665&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C104665&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>ie:</b>      | Ionization energy                               |
| <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>rlnpol:</b> | Non-polar retention indices         |
| <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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