

# Dibenzo-p-dioxin, 1,9-dichloro

|                      |                                                                          |
|----------------------|--------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C12H6Cl2O2/c13-7-3-1-5-9-11(7)16-12-8(14)4-2-6-10(12)15-9/h1-6H |
| InchiKey:            | JZDVJXBKJDADAY-UHFFFAOYSA-N                                              |
| Formula:             | C12H6Cl2O2                                                               |
| SMILES:              | Clc1cccc2c1Oc1c(Cl)cccc1O2                                               |
| Mol. weight [g/mol]: | 253.08                                                                   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 120.92  | kJ/mol  | Joback Method  |
| hf            | -60.01  | kJ/mol  | Joback Method  |
| hfus          | 36.88   | kJ/mol  | Joback Method  |
| hvap          | 67.35   | kJ/mol  | Joback Method  |
| log10ws       | -4.36   |         | Crippen Method |
| logp          | 4.891   |         | Crippen Method |
| mcvol         | 157.780 | ml/mol  | McGowan Method |
| pc            | 3372.36 | kPa     | Joback Method  |
| rinpol        | 1982.00 |         | NIST Webbook   |
| rinpol        | 1970.00 |         | NIST Webbook   |
| rinpol        | 1982.00 |         | NIST Webbook   |
| rinpol        | 1970.00 |         | NIST Webbook   |
| rinpol        | 1971.00 |         | NIST Webbook   |
| tb            | 683.14  | K       | Joback Method  |
| tc            | 945.37  | K       | Joback Method  |
| tf            | 466.60  | K       | Joback Method  |
| vc            | 0.598   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 357.63 | J/mol×K | 683.14          | Joback Method |
| cpg           | 400.86 | J/mol×K | 901.66          | Joback Method |
| cpg           | 393.51 | J/mol×K | 857.96          | Joback Method |
| cpg           | 385.63 | J/mol×K | 814.25          | Joback Method |
| cpg           | 377.11 | J/mol×K | 770.55          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 367.82    | J/mol×K | 726.84 | Joback Method |
| cpg   | 407.80    | J/mol×K | 945.37 | Joback Method |
| dvisc | 0.0005130 | Pa×s    | 683.14 | Joback Method |
| dvisc | 0.0005854 | Pa×s    | 647.05 | Joback Method |
| dvisc | 0.0006785 | Pa×s    | 610.96 | Joback Method |
| dvisc | 0.0008012 | Pa×s    | 574.87 | Joback Method |
| dvisc | 0.0009673 | Pa×s    | 538.78 | Joback Method |
| dvisc | 0.0011999 | Pa×s    | 502.69 | Joback Method |
| dvisc | 0.0015388 | Pa×s    | 466.60 | 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=R50412&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R50412&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                   |
| <b>vc:</b>      | Critical Volume                                 |

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