

# Dibenzodioxin, 1-bromo-, 3,7-dichloro-

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C12H5BrCl2O2/c13-8-3-7(15)5-11-12(8)17-9-2-1-6(14)4-10(9)16-11/h1-5H

DLYNLDOMUPAYBG-UHFFFAOYSA-N

C12H5BrCl2O2

Clc1ccc2c(c1)Oc1cc(Cl)cc(Br)c1O2

331.98

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 125.61  | kJ/mol  | Joback Method  |
| hf            | -45.15  | kJ/mol  | Joback Method  |
| hfus          | 41.77   | kJ/mol  | Joback Method  |
| hvap          | 74.44   | kJ/mol  | Joback Method  |
| log10ws       | -5.52   |         | Crippen Method |
| logp          | 5.654   |         | Crippen Method |
| mcvol         | 175.280 | ml/mol  | McGowan Method |
| pc            | 3594.25 | kPa     | Joback Method  |
| rinpol        | 2217.00 |         | NIST Webbook   |
| rinpol        | 2217.00 |         | NIST Webbook   |
| tb            | 754.28  | K       | Joback Method  |
| tc            | 1027.42 | K       | Joback Method  |
| tf            | 538.92  | K       | Joback Method  |
| vc            | 0.659   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 381.64    | J/mol×K | 754.28          | Joback Method |
| cpg           | 390.26    | J/mol×K | 799.80          | Joback Method |
| cpg           | 398.22    | J/mol×K | 845.33          | Joback Method |
| cpg           | 405.64    | J/mol×K | 890.85          | Joback Method |
| cpg           | 412.67    | J/mol×K | 936.37          | Joback Method |
| cpg           | 419.46    | J/mol×K | 981.90          | Joback Method |
| cpg           | 426.14    | J/mol×K | 1027.42         | Joback Method |
| dvisc         | 0.0012797 | Pa×s    | 538.92          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0010327 | Pa×s | 574.81 | Joback Method |
| dvisc | 0.0008547 | Pa×s | 610.71 | Joback Method |
| dvisc | 0.0007224 | Pa×s | 646.60 | Joback Method |
| dvisc | 0.0006214 | Pa×s | 682.49 | Joback Method |
| dvisc | 0.0005427 | Pa×s | 718.39 | Joback Method |
| dvisc | 0.0004801 | Pa×s | 754.28 | 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=R317210&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R317210&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>mccol:</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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