

# Ethane, 1,2-dibromo-1,2-dichloro-

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | 1,2-Dibromo-1,2-dichloroethane<br>1,2-Dichloro-1,2-dibromoethane |
| <b>Inchi:</b>               | InChI=1S/C2H2Br2Cl2/c3-1(5)2(4)6/h1-2H                           |
| <b>InchiKey:</b>            | RJMDFMUPJANPGX-UHFFFAOYSA-N                                      |
| <b>Formula:</b>             | C2H2Br2Cl2   |
| <b>SMILES:</b>              | ClC(Br)C(Cl)Br   |
| <b>Mol. weight [g/mol]:</b> | 256.75   |
| <b>CAS:</b>                 | 683-68-1   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -34.14  | kJ/mol               | Joback Method  |
| hf            | -73.99  | kJ/mol               | Joback Method  |
| hfus          | 12.85   | kJ/mol               | Joback Method  |
| hvap          | 40.91   | kJ/mol               | Joback Method  |
| log10ws       | -3.04   |                      | Crippen Method |
| logp          | 2.906   |                      | Crippen Method |
| mvol          | 98.520  | ml/mol               | McGowan Method |
| pc            | 5653.23 | kPa                  | Joback Method  |
| rinpol        | 1073.00 |                      | NIST Webbook   |
| rinpol        | 1073.00 |                      | NIST Webbook   |
| tb            | 468.20  | K                    | NIST Webbook   |
| tc            | 689.12  | K                    | Joback Method  |
| tf            | 261.74  | K                    | Joback Method  |
| vc            | 0.357   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 144.99 | J/mol×K | 689.12          | Joback Method |
| cpg           | 126.27 | J/mol×K | 451.46          | Joback Method |
| cpg           | 130.30 | J/mol×K | 491.07          | Joback Method |
| cpg           | 133.91 | J/mol×K | 530.68          | Joback Method |
| cpg           | 137.15 | J/mol×K | 570.29          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 140.05    | J/mol×K | 609.90 | Joback Method |
| cpg   | 142.65    | J/mol×K | 649.51 | Joback Method |
| dvisc | 0.0004569 | Paxs    | 451.46 | Joback Method |
| dvisc | 0.0049706 | Paxs    | 261.74 | Joback Method |
| dvisc | 0.0026949 | Paxs    | 293.36 | Joback Method |
| dvisc | 0.0016459 | Paxs    | 324.98 | Joback Method |
| dvisc | 0.0010971 | Paxs    | 356.60 | Joback Method |
| dvisc | 0.0007812 | Paxs    | 388.22 | Joback Method |
| dvisc | 0.0005855 | Paxs    | 419.84 | Joback Method |
| hvapt | 45.90     | kJ/mol  | 349.50 | NIST Webbook  |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.74227e+01                   |
| Coeff. B                    | -6.28397e+03                  |
| Coeff. C                    | 2.26160e+01                   |
| Temperature range (K), min. | 344.11                        |
| Temperature range (K), max. | 496.24                        |

## 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=C683681&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C683681&amp;Units=SI</a>   |
| <b>The Yaws Handbook of Vapor Pressure:</b> | <a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a> |
| <b>Crippen Method:</b>                      | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>hvapt:</b>   | Enthalpy of vaporization at a given temperature |
| <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>pvap:</b>    | Vapor pressure                                  |
| <b>rinp:</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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