

# Ethane, 1,1,2-tribromo-

|                      |                                     |
|----------------------|-------------------------------------|
| Other names:         | 1,1,2-Tribromoethane                |
| Inchi:               | InChI=1S/C2H3Br3/c3-1-2(4)5/h2H,1H2 |
| InchiKey:            | QUMDOMSJJIFTCA-UHFFFAOYSA-N         |
| Formula:             | C2H3Br3                             |
| SMILES:              | BrCC(Br)Br                          |
| Mol. weight [g/mol]: | 266.76                              |
| CAS:                 | 78-74-0                             |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 6.48    | kJ/mol  | Joback Method  |
| hf            | -10.90  | kJ/mol  | Joback Method  |
| hfus          | 13.27   | kJ/mol  | Joback Method  |
| hvap          | 38.96   | kJ/mol  | Joback Method  |
| log10ws       | -2.56   |         | Crippen Method |
| logp          | 2.497   |         | Crippen Method |
| mcvol         | 91.540  | ml/mol  | McGowan Method |
| pc            | 7002.68 | kPa     | Joback Method  |
| tb            | 443.20  | K       | Joback Method  |
| tc            | 680.89  | K       | Joback Method  |
| tf            | 276.70  | K       | Joback Method  |
| vc            | 0.328   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 113.82    | J/mol×K | 443.20          | Joback Method |
| cpg           | 131.33    | J/mol×K | 641.27          | Joback Method |
| cpg           | 128.51    | J/mol×K | 601.66          | Joback Method |
| cpg           | 125.40    | J/mol×K | 562.04          | Joback Method |
| cpg           | 121.94    | J/mol×K | 522.43          | Joback Method |
| cpg           | 118.09    | J/mol×K | 482.81          | Joback Method |
| cpg           | 133.88    | J/mol×K | 680.89          | Joback Method |
| dvisc         | 0.0004988 | Pa×s    | 443.20          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0006151 | Pa×s | 415.45 | Joback Method |
| dvisc | 0.0007817 | Pa×s | 387.70 | Joback Method |
| dvisc | 0.0010308 | Pa×s | 359.95 | Joback Method |
| dvisc | 0.0014235 | Pa×s | 332.20 | Joback Method |
| dvisc | 0.0020849 | Pa×s | 304.45 | Joback Method |
| dvisc | 0.0032967 | Pa×s | 276.70 | Joback Method |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.50765e+01                   |
| Coeff. B                    | -4.10474e+03                  |
| Coeff. C                    | -6.96080e+01                  |
| Temperature range (K), min. | 347.16                        |
| Temperature range (K), max. | 489.96                        |

## Sources

|                                      |                                                                                                                                                                                         |
|--------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 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>                                                                                   |
| KDB:                                 | <a href="https://www.thermo.com/files/research/kdb/mol/mol1564.mol">https://www.thermo.com/files/research/kdb/mol/mol1564.mol</a>                                                       |
| McGowan Method:                      | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                                                                   |
| NIST Webbook:                        | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C78740&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C78740&amp;Units=SI</a>                                                 |
| The Yaws Handbook of Vapor Pressure: | <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> |
| Crippen Method:                      | <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>h<sub>vap</sub>:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log<sub>10</sub>ws:</b> | Log10 of Water solubility in mol/l              |
| <b>log<sub>p</sub>:</b>    | Octanol/Water partition coefficient             |
| <b>mc<sub>vol</sub>:</b>   | McGowan's characteristic volume                 |
| <b>p<sub>c</sub>:</b>      | Critical Pressure                               |
| <b>p<sub>vap</sub>:</b>    | Vapor pressure                                  |
| <b>t<sub>b</sub>:</b>      | Normal Boiling Point Temperature                |
| <b>t<sub>c</sub>:</b>      | Critical Temperature                            |
| <b>t<sub>f</sub>:</b>      | Normal melting (fusion) point                   |
| <b>v<sub>c</sub>:</b>      | Critical Volume                                 |

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