

# bis-(2-Chloroethyl)trisulfide

|                      |  |
|----------------------|--|
| Inchi:               | InChI=1S/C4H8Cl2S3/c5-1-3-7-9-8-4-2-6/h1-4H2 |
| InchiKey:            | XHODIRQQNWHUGV-UHFFFAOYSA-N                  |
| Formula:             | C4H8Cl2S3                                    |
| SMILES:              | CICCSSSCCCI                                  |
| Mol. weight [g/mol]: | 223.21                                       |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 58.30   | kJ/mol               | Joback Method  |
| hf            | -31.76  | kJ/mol               | Joback Method  |
| hfus          | 26.90   | kJ/mol               | Joback Method  |
| hvap          | 53.72   | kJ/mol               | Joback Method  |
| log10ws       | -3.44   |                      | Crippen Method |
| logp          | 3.494   |                      | Crippen Method |
| mvol          | 140.750 | ml/mol               | McGowan Method |
| pc            | 3786.98 | kPa                  | Joback Method  |
| ripol         | 2456.00 |                      | NIST Webbook   |
| ripol         | 2456.00 |                      | NIST Webbook   |
| tb            | 572.12  | K                    | Joback Method  |
| tc            | 824.18  | K                    | Joback Method  |
| tf            | 297.88  | K                    | Joback Method  |
| vc            | 0.519   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 258.93 | J/molxK | 572.12          | Joback Method |
| cpg           | 267.98 | J/molxK | 614.13          | Joback Method |
| cpg           | 276.44 | J/molxK | 656.14          | Joback Method |
| cpg           | 284.30 | J/molxK | 698.15          | Joback Method |
| cpg           | 291.55 | J/molxK | 740.16          | Joback Method |
| cpg           | 298.17 | J/molxK | 782.17          | Joback Method |
| cpg           | 304.16 | J/molxK | 824.18          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |
| <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=R596171&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R596171&amp;Units=SI</a> |

# Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <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>ripol:</b>   | 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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