

# trithiacyclohexene

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C4H6S2/c1-2-4-6-5-3-1/h1,3H,2,4H2 |
| <b>InchiKey:</b>            | KRXAVBPUAIKSFF-UHFFFAOYSA-N                |
| <b>Formula:</b>             | C4H6S2                                     |
| <b>SMILES:</b>              | C1=CSSCC1                                  |
| <b>Mol. weight [g/mol]:</b> | 118.22                                     |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 124.64  | kJ/mol               | Joback Method  |
| hf            | 97.07   | kJ/mol               | Joback Method  |
| hfus          | 5.42    | kJ/mol               | Joback Method  |
| hvap          | 37.15   | kJ/mol               | Joback Method  |
| log10ws       | -2.50   |                      | Crippen Method |
| logp          | 2.285   |                      | Crippen Method |
| mcvol         | 84.760  | ml/mol               | McGowan Method |
| pc            | 5569.17 | kPa                  | Joback Method  |
| rinqol        | 1168.00 |                      | NIST Webbook   |
| tb            | 409.96  | K                    | Joback Method  |
| tc            | 659.97  | K                    | Joback Method  |
| tf            | 314.12  | K                    | Joback Method  |
| vc            | 0.272   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 133.22 | J/mol×K | 409.96          | Joback Method |
| cpg           | 143.76 | J/mol×K | 451.63          | Joback Method |
| cpg           | 153.52 | J/mol×K | 493.30          | Joback Method |
| cpg           | 162.54 | J/mol×K | 534.97          | Joback Method |
| cpg           | 170.86 | J/mol×K | 576.64          | Joback Method |
| cpg           | 178.53 | J/mol×K | 618.30          | Joback Method |
| cpg           | 185.58 | J/mol×K | 659.97          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <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>                                 |
| <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=R155032&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R155032&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>mccvol:</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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