

# 2,3,5,6-tetrathiaheptane

|                      |                                           |
|----------------------|-------------------------------------------|
| Inchi:               | InChI=1S/C3H8S4/c1-4-6-3-7-5-2/h3H2,1-2H3 |
| InchiKey:            | VDSAPPVDLHMMGQ-UHFFFAOYSA-N               |
| Formula:             | C3H8S4                                    |
| SMILES:              | CSSCSCC                                   |
| Mol. weight [g/mol]: | 172.36                                    |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 106.86  | kJ/mol  | Joback Method  |
| hf            | 62.23   | kJ/mol  | Joback Method  |
| hfus          | 20.05   | kJ/mol  | Joback Method  |
| hvap          | 49.54   | kJ/mol  | Joback Method  |
| log10ws       | -3.09   |         | Crippen Method |
| logp          | 2.966   |         | Crippen Method |
| mcvol         | 118.530 | ml/mol  | McGowan Method |
| pc            | 4835.95 | kPa     | Joback Method  |
| rinpol        | 1327.00 |         | NIST Webbook   |
| tb            | 543.16  | K       | Joback Method  |
| tc            | 815.04  | K       | Joback Method  |
| tf            | 261.17  | K       | Joback Method  |
| vc            | 0.419   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 215.81 | J/mol×K | 543.16          | Joback Method |
| cpg           | 225.24 | J/mol×K | 588.47          | Joback Method |
| cpg           | 234.13 | J/mol×K | 633.79          | Joback Method |
| cpg           | 242.44 | J/mol×K | 679.10          | Joback Method |
| cpg           | 250.12 | J/mol×K | 724.42          | Joback Method |
| cpg           | 257.12 | J/mol×K | 769.73          | Joback Method |
| cpg           | 263.40 | J/mol×K | 815.04          | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R217031&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R217031&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>                                 |
| <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>                     |

## 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>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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