

# Allyl methyl tetrasulfide

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | Methyl 2-propenyl tetrasulfide                 |
| <b>Inchi:</b>               | InChI=1S/C4H8S4/c1-3-4-6-8-7-5-2/h3H,1,4H2,2H3 |
| <b>InchiKey:</b>            | BHIKXWJMZCALEK-UHFFFAOYSA-N                    |
| <b>Formula:</b>             | C4H8S4   |
| <b>SMILES:</b>              | C=CCSSSSC                                      |
| <b>Mol. weight [g/mol]:</b> | 184.37   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 203.12  | kJ/mol               | Joback Method  |
| hf            | 167.02  | kJ/mol               | Joback Method  |
| hfus          | 21.36   | kJ/mol               | Joback Method  |
| hvap          | 51.10   | kJ/mol               | Joback Method  |
| log10ws       | -3.86   |                      | Crippen Method |
| logp          | 3.480   |                      | Crippen Method |
| mcvol         | 128.320 | ml/mol               | McGowan Method |
| pc            | 4492.23 | kPa                  | Joback Method  |
| rinpol        | 1386.00 |                      | NIST Webbook   |
| rinpol        | 1355.00 |                      | NIST Webbook   |
| rinpol        | 1386.00 |                      | NIST Webbook   |
| rinpol        | 1358.00 |                      | NIST Webbook   |
| rinpol        | 1325.00 |                      | NIST Webbook   |
| rinpol        | 1322.00 |                      | NIST Webbook   |
| rinpol        | 1355.00 |                      | NIST Webbook   |
| rinpol        | 1325.00 |                      | NIST Webbook   |
| rinpol        | 1322.00 |                      | NIST Webbook   |
| tb            | 562.72  | K                    | Joback Method  |
| tc            | 834.71  | K                    | Joback Method  |
| tf            | 270.68  | K                    | Joback Method  |
| vc            | 0.457   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-------|------|-----------------|--------|
|---------------|-------|------|-----------------|--------|

|     |        |         |        |               |
|-----|--------|---------|--------|---------------|
| cpg | 238.98 | J/mol×K | 562.72 | Joback Method |
| cpg | 248.85 | J/mol×K | 608.05 | Joback Method |
| cpg | 258.06 | J/mol×K | 653.38 | Joback Method |
| cpg | 266.59 | J/mol×K | 698.72 | Joback Method |
| cpg | 274.40 | J/mol×K | 744.05 | Joback Method |
| cpg | 281.47 | J/mol×K | 789.38 | Joback Method |
| cpg | 287.75 | J/mol×K | 834.71 | 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=R53418&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R53418&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>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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