

# 3,6-Di-isopropyl-[1,2,4,5]tetrathiane

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C8H16S4/c1-5(2)7-9-11-8(6(3)4)12-10-7/h5-8H,1-4H3

ROBADD CVLNSGOK-UHFFFAOYSA-N

C8H16S4

CC(C)C1SSC(C(C)C)SS1

240.47

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 187.78  | kJ/mol  | Joback Method  |
| hf            | -3.99   | kJ/mol  | Joback Method  |
| hfus          | 16.96   | kJ/mol  | Joback Method  |
| hvap          | 55.99   | kJ/mol  | Joback Method  |
| log10ws       | -5.31   |         | Crippen Method |
| logp          | 4.727   |         | Crippen Method |
| mcvol         | 178.120 | ml/mol  | McGowan Method |
| pc            | 3012.33 | kPa     | Joback Method  |
| ripol         | 2130.00 |         | NIST Webbook   |
| ripol         | 2130.00 |         | NIST Webbook   |
| tb            | 587.76  | K       | Joback Method  |
| tc            | 856.46  | K       | Joback Method  |
| tf            | 486.86  | K       | Joback Method  |
| vc            | 0.588   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 407.06 | J/mol×K | 587.76          | Joback Method |
| cpg           | 425.32 | J/mol×K | 632.54          | Joback Method |
| cpg           | 442.27 | J/mol×K | 677.33          | Joback Method |
| cpg           | 457.94 | J/mol×K | 722.11          | Joback Method |
| cpg           | 472.41 | J/mol×K | 766.89          | Joback Method |
| cpg           | 485.71 | J/mol×K | 811.67          | Joback Method |
| cpg           | 497.91 | J/mol×K | 856.46          | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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=R495211&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R495211&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>                                 |

# 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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