

# Rhodanine, 5,5'-ethylenedi-

**Inchi:** InChI=1S/C8H8N2O2S4/c1-2(3-5(11)9-7(13)15-3)4-6(12)10-8(14)16-4/h2-4H,1H3,(H,9,1  
**InchiKey:** CAXCSMMWQXAWSL-UHFFFAOYSA-N  
**Formula:** C8H8N2O2S4  
**SMILES:** CC(C1SC(=S)NC1=O)C1SC(=S)NC1=O  
**Mol. weight [g/mol]:** 292.42

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 278.80  | kJ/mol  | Joback Method  |
| hf            | 28.17   | kJ/mol  | Joback Method  |
| hfus          | 38.40   | kJ/mol  | Joback Method  |
| hvap          | 82.12   | kJ/mol  | Joback Method  |
| log10ws       | -3.33   |         | Crippen Method |
| logp          | 0.655   |         | Crippen Method |
| mcvol         | 181.760 | ml/mol  | McGowan Method |
| pc            | 5235.81 | kPa     | Joback Method  |
| tb            | 886.24  | K       | Joback Method  |
| tc            | 1208.21 | K       | Joback Method  |
| tf            | 827.46  | K       | Joback Method  |
| vc            | 0.616   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 474.12 | J/mol×K | 886.24          | Joback Method |
| cpg           | 485.36 | J/mol×K | 939.90          | Joback Method |
| cpg           | 495.03 | J/mol×K | 993.56          | Joback Method |
| cpg           | 503.15 | J/mol×K | 1047.22         | Joback Method |
| cpg           | 509.70 | J/mol×K | 1100.89         | Joback Method |
| cpg           | 514.70 | J/mol×K | 1154.55         | Joback Method |
| cpg           | 518.16 | J/mol×K | 1208.21         | Joback Method |

# Sources

|                        |                                                                                                                                             |
|------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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=B6000725&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6000725&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>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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