

# Carbonodithioic acid, O,S-dimethyl ester

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | Carbonic acid, dithio-, O,S-dimethyl ester<br>Dimethyl xanthate<br>Methyl O-methylxanthate<br>Methyl S-methyl xanthate<br>O-Methyl S-methyl dithiocarbonate<br>O,S-Dimethyl dithiocarbonate |
| <b>Inchi:</b>               | InChI=1S/C3H6OS2/c1-4-3(5)6-2/h1-2H3  |
| <b>InchiKey:</b>            | LABVNFAVENLDHB-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C3H6OS2   |
| <b>SMILES:</b>              | COC(=S)SC   |
| <b>Mol. weight [g/mol]:</b> | 122.21  |
| <b>CAS:</b>                 | 19708-81-7  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 19.56   | kJ/mol               | Joback Method  |
| hf            | -49.10  | kJ/mol               | Joback Method  |
| hfus          | 13.45   | kJ/mol               | Joback Method  |
| hvap          | 38.23   | kJ/mol               | Joback Method  |
| log10ws       | -1.40   |                      | Crippen Method |
| logp          | 1.281   |                      | Crippen Method |
| mcvol         | 87.400  | ml/mol               | McGowan Method |
| pc            | 5001.51 | kPa                  | Joback Method  |
| tb            | 429.28  | K                    | Joback Method  |
| tc            | 655.19  | K                    | Joback Method  |
| tf            | 214.47  | K                    | Joback Method  |
| vc            | 0.311   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 145.29 | J/mol×K | 429.28          | Joback Method |
| cpg           | 151.98 | J/mol×K | 466.93          | Joback Method |
| cpg           | 158.31 | J/mol×K | 504.58          | Joback Method |

|     |        |         |        |               |
|-----|--------|---------|--------|---------------|
| cpg | 164.27 | J/mol×K | 542.23 | Joback Method |
| cpg | 169.89 | J/mol×K | 579.88 | Joback Method |
| cpg | 175.19 | J/mol×K | 617.54 | Joback Method |
| cpg | 180.18 | J/mol×K | 655.19 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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=C19708817&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C19708817&amp;Units=SI</a> |
| <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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>   |

## 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>h vap:</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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