

# Disulfide, bis(2-nitrophenyl)

|                             |                                                                                                                                                                                                                                                                     |
|-----------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Other names:</b>         | Disulfide, bis(o-nitrophenyl)<br>O,O'-Dinitrodiphenyl disulfide<br>Bis(o-nitrophenyl) disulfide<br>Bis(2-nitrophenyl) disulfide<br>2,2'-Dinitrodiphenyl disulfide<br>2-Nitrophenyl disulfide<br>o-Nitrophenyl disulfide<br>NSC 203<br>bis(2-nitrophenyl) disulphide |
| <b>Inchi:</b>               | InChI=1S/C12H8N2O4S2/c15-13(16)9-5-1-3-7-11(9)19-20-12-8-4-2-6-10(12)14(17)18/h                                                                                                                                                                                     |
| <b>InchiKey:</b>            | NXCKJENHTITELM-UHFFFAOYSA-N                                                                                                                                                                                                                                         |
| <b>Formula:</b>             | C12H8N2O4S2                                                                                                                                                                                                                                                         |
| <b>SMILES:</b>              | O=[N+](O)c1cccc1SSc1cccc1[N+](=O)[O-]                                                                                                                                                                                                                               |
| <b>Mol. weight [g/mol]:</b> | 308.33                                                                                                                                                                                                                                                              |
| <b>CAS:</b>                 | 1155-00-6                                                                                                                                                                                                                                                           |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 393.06  | kJ/mol  | Joback Method  |
| hf            | 221.33  | kJ/mol  | Joback Method  |
| hfus          | 45.12   | kJ/mol  | Joback Method  |
| hvap          | 95.00   | kJ/mol  | Joback Method  |
| log10ws       | -6.06   |         | Crippen Method |
| logp          | 4.302   |         | Crippen Method |
| mcvol         | 199.960 | ml/mol  | McGowan Method |
| pc            | 3543.08 | kPa     | Joback Method  |
| tb            | 978.52  | K       | Joback Method  |
| tc            | 1295.96 | K       | Joback Method  |
| tf            | 658.90  | K       | Joback Method  |
| vc            | 0.763   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

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

|     |        |         |         |               |
|-----|--------|---------|---------|---------------|
| cpg | 537.82 | J/mol×K | 978.52  | Joback Method |
| cpg | 545.01 | J/mol×K | 1031.43 | Joback Method |
| cpg | 550.69 | J/mol×K | 1084.33 | Joback Method |
| cpg | 554.95 | J/mol×K | 1137.24 | Joback Method |
| cpg | 557.90 | J/mol×K | 1190.15 | Joback Method |
| cpg | 559.65 | J/mol×K | 1243.05 | Joback Method |
| cpg | 560.29 | J/mol×K | 1295.96 | 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=C1155006&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1155006&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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