

# 4-Amino-6-chlorobenzene-1,3-disulfonamide

|                      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
|----------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 5-Chloro-2,4-disulfamylaniline<br>m-Chloroaniline-4,6-disulfonamide<br>1-Amino-3-chloro-4,6-benzenedisulfonamide<br>1,3-Benzenedisulfonamide, 4-amino-6-chloro-<br>m-Benzenedisulfonamide, 4-amino-6-chloro-<br>Chloraminophenamide<br>Chloroaminophenamide<br>Idorese<br>Salamid<br>Salmid<br>Su 5683<br>3-Chloro-4,6-disulfamoylaniline<br>4-Amino-6-chloro-m-benzenedisulfonamide<br>5-Chloro-2,4-disulfamoylaniline<br>4-Amino-6-chloro-1,3-benzenedisulfonamide<br>1,3-Disulfonamide, 4-amino-6-chlorobenzene-<br>4-amino-6-chlorobenzene-1,3-disulphonamide |
| Inchi:               | InChI=1S/C6H8ClN3O4S2/c7-3-1-4(8)6(16(10,13)14)2-5(3)15(9,11)12/h1-2H,8H2,(H2,9,                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
| InchiKey:            | IHJCXVZDYSXXFT-UHFFFAOYSA-N                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| Formula:             | C6H8ClN3O4S2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| SMILES:              | Nc1cc(Cl)c(S(N)(=O)=O)cc1S(N)(=O)=O                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| Mol. weight [g/mol]: | 285.73                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
| CAS:                 | 121-30-2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| gf            | -666.50 | kJ/mol | Joback Method  |
| hf            | -786.12 | kJ/mol | Joback Method  |
| hfus          | 46.71   | kJ/mol | Joback Method  |
| hvap          | 106.79  | kJ/mol | Joback Method  |
| log10ws       | -1.19   |        | Crippen Method |
| logp          | -0.783  |        | Crippen Method |
| mcvol         | 170.000 | ml/mol | McGowan Method |
| pc            | 8833.17 | kPa    | Joback Method  |
| tb            | 728.88  | K      | Joback Method  |
| tc            | 962.82  | K      | Joback Method  |
| tf            | 578.18  | K      | Joback Method  |

|    |       |                      |               |
|----|-------|----------------------|---------------|
| vc | 0.651 | m <sup>3</sup> /kmol | Joback Method |
|----|-------|----------------------|---------------|

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 415.95 | J/mol×K | 728.88          | Joback Method |
| cpg           | 424.72 | J/mol×K | 767.87          | Joback Method |
| cpg           | 432.52 | J/mol×K | 806.86          | Joback Method |
| cpg           | 439.32 | J/mol×K | 845.85          | Joback Method |
| cpg           | 445.09 | J/mol×K | 884.84          | Joback Method |
| cpg           | 449.80 | J/mol×K | 923.83          | Joback Method |
| cpg           | 453.44 | J/mol×K | 962.82          | Joback Method |

## Sources

|                 |                                                                                                                                           |
|-----------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| Joback Method:  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C121302&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C121302&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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                   |

**vc:** Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/17-863-5/4-Amino-6-chlorobenzene-1-3-disulfonamide.pdf>

Generated by Cheméo on 2025-12-23 02:26:19.506321198 +0000 UTC m=+6204977.036361864.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.