

# Ethanol, 2,2'-((m-chlorophenyl)imino)di-

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | N-(3-Chlorophenyl)-2,2'-iminodiethanol<br>N,N-Dihydroxyethyl-m-chloroaniline<br>N,N-Bis(2-hydroxyethyl)-m-chloroaniline<br>Ethanol, 2,2'-[(3-chlorophenyl)imino]bis-(m-Chlorophenyl)diethanolamine<br>m-Chloro-N,N-bis(2-hydroxyethyl)aniline<br>Aniline, m-chloro-N,N-bis(2-hydroxyethyl)-<br>Aniline, m-chloro-N,N-dihydroxyethyl-<br>Ethanol, 2,2'-(m-chloroanilino)bis-<br>N-(m-Chlorophenyl)diethanolamine<br>N-(3-Chlorophenyl)diethanolamine<br>N,N-Bis(2-hydroxyethyl)-3-chloroaniline<br>N,N-Di(«beta»-hydroxyethyl)-m-chloroaniline<br>2,2'-(m-chlorophenylimino)diethanol<br>3-Chloro-N,N-bis(2-hydroxyethyl)aniline<br>N,N-Bis(2-hydroxyethyl)chloroanilide<br>Diethanolaminochlorobenzene<br>N,N-Dihydroxyethyl-3-chloroaniline<br>Emery 5715<br>Emery 5717<br>NSC 58170<br>2,2'-(3-chlorophenylimino)diethanol |
| <b>Inchi:</b>               | InChI=1S/C10H14ClNO2/c11-9-2-1-3-10(8-9)12(4-6-13)5-7-14/h1-3,8,13-14H,4-7H2   |
| <b>InchiKey:</b>            | MVQUJEUCFOGFJU-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C10H14ClNO2  |
| <b>SMILES:</b>              | OCCN(CCO)c1cccc(Cl)c1  |
| <b>Mol. weight [g/mol]:</b> | 215.68   |
| <b>CAS:</b>                 | 92-00-2  |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| gf            | -38.69  | kJ/mol | Joback Method  |
| hf            | -277.34 | kJ/mol | Joback Method  |
| hfus          | 30.70   | kJ/mol | Joback Method  |
| hvap          | 80.58   | kJ/mol | Joback Method  |
| log10ws       | -1.43   |        | Crippen Method |

|      |         |                      |                |
|------|---------|----------------------|----------------|
| logp | 1.131   |                      | Crippen Method |
| mvol | 161.960 | ml/mol               | McGowan Method |
| pc   | 3392.03 | kPa                  | Joback Method  |
| tb   | 694.09  | K                    | Joback Method  |
| tc   | 880.89  | K                    | Joback Method  |
| tf   | 425.43  | K                    | Joback Method  |
| vc   | 0.593   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 422.46 | J/mol×K | 694.09          | Joback Method |
| cpg           | 432.27 | J/mol×K | 725.22          | Joback Method |
| cpg           | 441.50 | J/mol×K | 756.36          | Joback Method |
| cpg           | 450.18 | J/mol×K | 787.49          | Joback Method |
| cpg           | 458.35 | J/mol×K | 818.62          | Joback Method |
| cpg           | 466.03 | J/mol×K | 849.76          | Joback Method |
| cpg           | 473.26 | J/mol×K | 880.89          | 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=C92002&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C92002&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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