

# 1-Chlorobenzene, 4-(4-bromobenzylidenamino)-

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | N-[(4-Bromophenyl)methylidene]-4-chloroaniline<br>p-Bromobenzylidene-(4-chlorophenyl)-amine<br>Benzenamine, N-[(4-bromophenyl)methylene]-4-chloro- |
| <b>Inchi:</b>               | InChI=1S/C13H9BrClN/c14-11-3-1-10(2-4-11)9-16-13-7-5-12(15)6-8-13/h1-9H  |
| <b>InchiKey:</b>            | HYGUYDRZPYYAMJ-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C13H9BrClN   |
| <b>SMILES:</b>              | Clc1ccc(N=Cc2ccc(Br)cc2)cc1  |
| <b>Mol. weight [g/mol]:</b> | 294.57   |
| <b>CAS:</b>                 | 55327-54-3   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hf            | 231.28  | kJ/mol | Joback Method  |
| hvap          | 64.54   | kJ/mol | Joback Method  |
| log10ws       | -5.19   |        | Crippen Method |
| logp          | 4.853   |        | Crippen Method |
| mcvol         | 181.930 | ml/mol | McGowan Method |
| pc            | 2749.78 | kPa    | Joback Method  |
| rinpola       | 2289.00 |        | NIST Webbook   |
| tb            | 740.43  | K      | Joback Method  |
| tc            | 1016.66 | K      | 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=C55327543&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C55327543&amp;Units=SI</a> |

# Legend

|                            |   |
|----------------------------|---|
| <b>hf:</b>                 | Enthalpy of formation at standard conditions    |
| <b>h<sub>vap</sub>:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log<sub>10</sub>ws:</b> | Log <sub>10</sub> of Water solubility in mol/l  |
| <b>log<sub>p</sub>:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>              | McGowan's characteristic volume                 |
| <b>pc:</b>                 | Critical Pressure                               |
| <b>r<sub>inpol</sub>:</b>  | Non-polar retention indices                     |
| <b>tb:</b>                 | Normal Boiling Point Temperature                |
| <b>tc:</b>                 | Critical Temperature                            |

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