

# Benzenamine, 5-chloro-2-methyl-

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | o-Toluidine, 5-chloro-<br>Acco Fast Red KB base<br>Ansibase Red KB<br>Azoene Fast Red KB base<br>Fast Red KB amine<br>Fast Red KB salt<br>Fast Red KB salt Supra<br>Fast Red KB Base<br>Fast Red KBS salt<br>Genazo Red KB soln<br>Hiltonil Fast Red KB base<br>Lake Red BK base<br>Metrogen Red Former KB soln<br>Naphthosol Fast Red KB base<br>Pharmazoid Red KB<br>Red KB base<br>Spectrolene Red KB<br>Stable Red KB base<br>2-Amino-4-chlorotoluene<br>2-Methyl-5-chloroaniline<br>3-Chloro-6-methylaniline<br>5-Chloro-o-toluidine<br>5-Chloro-2-methylaniline<br>5-Chloro-ortho-toluidine<br>4-Chloro-2-aminotoluene<br>Azoic diazo component 32<br>Azoic diazo component 32, base<br>C.I. Azoic Diazo Component 32<br>NCI-C02051<br>1-Amino-3-chloro-6-methylbenzene<br>5-Chloro-2-methylbenzenamine<br>5-Chloro-2-toluidine<br>Fast Red KB-T Base<br>NSC 7094 |
| <b>Inchi:</b>               | InChI=1S/C7H8ClN/c1-5-2-3-6(8)4-7(5)9/h2-4H,9H2,1H3   |
| <b>InchiKey:</b>            | WRZOMWDJOLIVQP-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C7H8ClN   |
| <b>SMILES:</b>              | <chem>Cc1ccc(Cl)cc1N</chem>   |
| <b>Mol. weight [g/mol]:</b> | 141.60  |
| <b>CAS:</b>                 | 95-79-4   |

# Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 155.73  | kJ/mol               | Joback Method  |
| hf            | 43.83   | kJ/mol               | Joback Method  |
| hfus          | 16.54   | kJ/mol               | Joback Method  |
| hvap          | 49.80   | kJ/mol               | Joback Method  |
| log10ws       | -2.27   |                      | Crippen Method |
| logp          | 2.231   |                      | Crippen Method |
| mcvol         | 107.950 | ml/mol               | McGowan Method |
| pc            | 4062.13 | kPa                  | Joback Method  |
| rinpol        | 1261.50 |                      | NIST Webbook   |
| rinpol        | 1256.00 |                      | NIST Webbook   |
| rinpol        | 1256.00 |                      | NIST Webbook   |
| rinpol        | 1256.00 |                      | NIST Webbook   |
| rinpol        | 1261.50 |                      | NIST Webbook   |
| ripol         | 2145.00 |                      | NIST Webbook   |
| ripol         | 2145.00 |                      | NIST Webbook   |
| ripol         | 2145.00 |                      | NIST Webbook   |
| tb            | 510.20  | K                    | NIST Webbook   |
| tc            | 741.33  | K                    | Joback Method  |
| tf            | 333.29  | K                    | Joback Method  |
| vc            | 0.398   | m <sup>3</sup> /kmol | Joback Method  |

# Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 211.08 | J/mol×K | 506.16          | Joback Method |
| cpg           | 221.33 | J/mol×K | 545.35          | Joback Method |
| cpg           | 230.94 | J/mol×K | 584.55          | Joback Method |
| cpg           | 239.95 | J/mol×K | 623.74          | Joback Method |
| cpg           | 248.37 | J/mol×K | 662.94          | Joback Method |
| cpg           | 256.22 | J/mol×K | 702.13          | Joback Method |
| cpg           | 263.54 | J/mol×K | 741.33          | Joback Method |

# Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 510.20 | K    | 96.30          | NIST Webbook |

## Sources

|                 |   |
|-----------------|---|
| 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=C95794&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C95794&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>                       |
| Joback Method:  | <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>hvp:</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>rinpol:</b>  | Non-polar retention indices                     |
| <b>ripol:</b>   | Polar retention indices                         |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tbrp:</b>    | Boiling point at reduced pressure               |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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