

# Borane, dichlorophenyl-

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | Dichlorophenylborane<br>Phenylboron dichloride<br>Phenyldichloroborane<br>Dichlorophenylboron |
| <b>Inchi:</b>               | InChI=1S/C6H5BCl2/c8-7(9)6-4-2-1-3-5-6/h1-5H  |
| <b>InchiKey:</b>            | NCQDQONETMHUMY-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C6H5BCl2  |
| <b>SMILES:</b>              | ClB(Cl)c1ccccc1   |
| <b>Mol. weight [g/mol]:</b> | 158.82  |
| <b>CAS:</b>                 | 873-51-8  |

## Physical Properties

| Property code | Value | Unit | Source         |
|---------------|-------|------|----------------|
| ie            | 9.30  | eV   | NIST Webbook   |
| ie            | 9.52  | eV   | NIST Webbook   |
| log10ws       | -4.39 |      | Crippen Method |
| logp          | 1.859 |      | Crippen Method |

## Temperature Dependent Properties

| Property code | Value        | Unit   | Temperature [K] | Source       |
|---------------|--------------|--------|-----------------|--------------|
| hvapt         | 33.70 ± 0.80 | kJ/mol | 295.50          | NIST Webbook |

## 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>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C873518&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C873518&amp;Units=SI</a> |

# Legend

|                 |   |
|-----------------|---|
| <b>hvapt:</b>   | Enthalpy of vaporization at a given temperature |
| <b>ie:</b>      | Ionization energy                               |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |

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