

# Borane, tributyl-

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | Tri-n-butylborane<br>Tri-n-butylboron<br>Tributylborane<br>Tributylboron<br>TBB<br>Tributylborine |
| <b>Inchi:</b>               | InChI=1S/C12H27B/c1-4-7-10-13(11-8-5-2)12-9-6-3/h4-12H2,1-3H3                                     |
| <b>InchiKey:</b>            | CMHHITPYCHHOGT-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C12H27B   |
| <b>SMILES:</b>              | CCCCB(CCCC)CCCC   |
| <b>Mol. weight [g/mol]:</b> | 182.15  |
| <b>CAS:</b>                 | 122-56-5  |

## Physical Properties

| Property code | Value | Unit | Source         |
|---------------|-------|------|----------------|
| log10ws       | -2.35 |      | Crippen Method |
| logp          | 4.881 |      | Crippen Method |

## Temperature Dependent Properties

| Property code | Value | Unit   | Temperature [K] | Source       |
|---------------|-------|--------|-----------------|--------------|
| hvapt         | 54.70 | kJ/mol | 328.00          | 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=C122565&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C122565&amp;Units=SI</a> |

# Legend

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

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