

# 4-Bromophenol, trimethylsilyl ether

|                      |                                                                                                                                                                                                                 |
|----------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 4-Trimethylsilyloxybromobenzene<br>4-Bromotrimethylsiloxybenzene<br>p-Bromophenoxytrimethylsilane<br>p-Trimethylsiloxy bromobenzene<br>(4-Bromophenoxy)(trimethyl)silane<br>4-Bromophenol, trimethylsilyl ether |
| Inchi:               | InChI=1S/C9H13BrOSi/c1-12(2,3)11-9-6-4-8(10)5-7-9/h4-7H,1-3H3                                                                                                                                                   |
| InchiKey:            | HWKPTBHJWBSOOP-UHFFFAOYSA-N                                                                                                                                                                                     |
| Formula:             | C9H13BrOSi                                                                                                                                                                                                      |
| SMILES:              | C[Si](C)(C)Oc1ccc(Br)cc1                                                                                                                                                                                        |
| Mol. weight [g/mol]: | 245.19                                                                                                                                                                                                          |

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| hvap          | 58.42   | kJ/mol | Cheméo Relay (1.0) |
| ie            | 8.69    | eV     | Cheméo Relay (1.0) |
| log10ws       | -3.50   |        | Cheméo Relay (1.0) |
| logp          | 3.663   |        | Crippen Method     |
| rinpol        | 1330.60 |        | NIST Webbook       |
| tb            | 518.65  | K      | Cheméo Relay (1.0) |
| tf            | 299.43  | K      | Cheméo Relay (1.0) |

## Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 399.00 | K    | 3.30           | NIST Webbook |

## Sources

|                 |                                                                                                                                               |
|-----------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C17878443&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C17878443&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:

[https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>ie:</b>      | Ionization energy                               |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>rinpol:</b>  | Non-polar retention indices                     |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tbrp:</b>    | Boiling point at reduced pressure               |
| <b>tf:</b>      | Normal melting (fusion) point                   |

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