# 2-Bromobenzenesulphonyl chloride

**Other names:** Benzenesulfonyl chloride, 2-bromo-
**Inchi:** InChI=1S/C6H4BrClO2S/c7-5-3-1-2-4-6(5)11(8,9)10/h1-4H
**InchiKey:** VFPWGZNNRSQPBT-UHFFFAOYSA-N
**Formula:** C6H4BrClO2S
**SMILES:** O=S(=O)(Cl)c1ccccc1Br
**Mol. weight [g/mol]:** 255.52

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hfus | 25.81 | kJ/mol | Joback Method |
| ie | 9.55 | eV | Cheméo Relay (1.0) |
| log10ws | -3.58 | | Cheméo Relay (1.0) |
| logp | 2.377 | | Crippen Method |
| mcvol | 129.470 | ml/mol | McGowan Method |
| tb | 567.65 | K | Cheméo Relay (1.0) |
| tf | 332.77 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 225.86 | J/mol×K | 519.71 | Joback Method |
| cpg | 234.97 | J/mol×K | 558.72 | Joback Method |
| cpg | 243.40 | J/mol×K | 597.72 | Joback Method |
| cpg | 251.16 | J/mol×K | 636.73 | Joback Method |
| cpg | 258.26 | J/mol×K | 675.74 | Joback Method |
| cpg | 264.72 | J/mol×K | 714.74 | Joback Method |
| cpg | 270.56 | J/mol×K | 753.75 | Joback Method |

## Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

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| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C2905251&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **tb:** | Normal Boiling Point Temperature |
| **tf:** | Normal melting (fusion) point |