# 3-Bromothiophenol

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|---|---|
| **Other names:** | m-Bromothiophenol |
| | Benzenethiol, 3-bromo- |
| | m-bromobenzenethiol |
| **Inchi:** | InChI=1S/C6H5BrS/c7-5-2-1-3-6(8)4-5/h1-4,8H |
| **InchiKey:** | HNGQQUDFJDROPY-UHFFFAOYSA-N |
| **Formula:** | C6H5BrS |
| **SMILES:** | Sc1cccc(Br)c1 |
| **Mol. weight [g/mol]:** | 189.07 |
| **CAS:** | 6320-01-0 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 146.13 | kJ/mol | Joback Method |
| hf | 122.70 | kJ/mol | Joback Method |
| hfus | 14.28 | kJ/mol | Joback Method |
| hvap | 45.06 | kJ/mol | Joback Method |
| log10ws | -3.15 | | Crippen Method |
| logp | 2.738 | | Crippen Method |
| mcvol | 105.490 | ml/mol | McGowan Method |
| pc | 5527.84 | kPa | Joback Method |
| tb | 497.36 | K | Joback Method |
| tc | 761.63 | K | Joback Method |
| tf | 292.58 | K | Joback Method |
| vc | 0.380 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 173.21 | J/mol×K | 497.36 | Joback Method |
| cpg | 182.36 | J/mol×K | 541.40 | Joback Method |
| cpg | 190.75 | J/mol×K | 585.45 | Joback Method |
| cpg | 198.42 | J/mol×K | 629.49 | Joback Method |
| cpg | 205.42 | J/mol×K | 673.54 | Joback Method |
| cpg | 211.82 | J/mol×K | 717.58 | Joback Method |

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|---|---|---|---|---|
| cpg | 217.66 | J/mol×K | 761.63 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 393.00 ± 1.00 | K | 2.80 | NIST Webbook |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C6320010&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**Joback Method:** https://en.wikipedia.org/wiki/Joback_method
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

# Legend

**cpg:** Ideal gas heat capacity
**gf:** Standard Gibbs free energy of formation
**hf:** Enthalpy of formation at standard conditions
**hfus:** Enthalpy of fusion at standard conditions
**hvap:** Enthalpy of vaporization at standard conditions
**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume
**pc:** Critical Pressure
**tb:** Normal Boiling Point Temperature
**tbrp:** Boiling point at reduced pressure
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point
**vc:** Critical Volume

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