# 4-Bromo-3-nitrobenzene sulfonic acid

**Inchi:** InChI=1S/C6H4BrNO5S/c7-5-2-1-4(14(11,12)13)3-6(5)8(9)10/h1-3H,(H,11,12,13)
**InchiKey:** LKQYUJYPYBCDOA-UHFFFAOYSA-N
**Formula:** C6H4BrNO5S
**SMILES:** O=[N+]([O-])c1cc(S(=O)(=O)O)ccc1Br
**Mol. weight [g/mol]:** 282.07
**CAS:** 584-49-6

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -462.70 | kJ/mol | Joback Method |
| hf | -543.59 | kJ/mol | Joback Method |
| hfus | 36.67 | kJ/mol | Joback Method |
| hvap | 90.89 | kJ/mol | Joback Method |
| log10ws | -2.87 | | Crippen Method |
| logp | 1.604 | | Crippen Method |
| mcvol | 140.520 | ml/mol | McGowan Method |
| pc | 7367.98 | kPa | Joback Method |
| tb | 731.28 | K | Joback Method |
| tc | 965.31 | K | Joback Method |
| tf | 511.63 | K | Joback Method |
| vc | 0.552 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 315.40 | J/mol×K | 731.28 | Joback Method |
| cpg | 322.05 | J/mol×K | 770.28 | Joback Method |
| cpg | 328.01 | J/mol×K | 809.29 | Joback Method |
| cpg | 333.28 | J/mol×K | 848.29 | Joback Method |
| cpg | 337.87 | J/mol×K | 887.30 | Joback Method |
| cpg | 341.80 | J/mol×K | 926.30 | Joback Method |
| cpg | 345.08 | J/mol×K | 965.31 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C584496&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 |

# Legend

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|---|---|
| **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 |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |