# 5-Amino-2-bromobenzotrifluoride

**Other names:** Benzenamine, 4-bromo-3-(trifluoromethyl)-
4-Bromo-«alpha»,«alpha»,«alpha»-trifluoro-m-toluidine
3-Trifluoromethyl-4-bromoaniline
**Inchi:** InChI=1S/C7H5BrF3N/c8-6-2-1-4(12)3-5(6)7(9,10)11/h1-3H,12H2
**InchiKey:** YGNISOAUPSJDJE-UHFFFAOYSA-N
**Formula:** C7H5BrF3N
**SMILES:** Nc1ccc(Br)c(C(F)(F)F)c1
**Mol. weight [g/mol]:** 240.02
**CAS:** 393-36-2

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -399.61 | kJ/mol | Joback Method |
| hf | -511.18 | kJ/mol | Joback Method |
| hfus | 19.46 | kJ/mol | Joback Method |
| hvap | 48.11 | kJ/mol | Joback Method |
| log10ws | -3.37 | | Crippen Method |
| logp | 3.050 | | Crippen Method |
| mcvol | 118.520 | ml/mol | McGowan Method |
| pc | 4010.84 | kPa | Joback Method |
| tb | 529.47 | K | Joback Method |
| tc | 753.19 | K | Joback Method |
| tf | 367.36 | K | Joback Method |
| vc | 0.454 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 248.96 | J/mol×K | 529.47 | Joback Method |
| cpg | 258.25 | J/mol×K | 566.76 | Joback Method |
| cpg | 266.76 | J/mol×K | 604.04 | Joback Method |
| cpg | 274.55 | J/mol×K | 641.33 | Joback Method |
| cpg | 281.67 | J/mol×K | 678.62 | Joback Method |
| cpg | 288.17 | J/mol×K | 715.91 | Joback Method |

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|---|---|---|---|---|
| cpg | 294.12 | J/mol×K | 753.19 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C393362&Units=SI |

# 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 |