# 4,4,4-Trifluoro-1-bromobutane

**Inchi:** InChI=1S/C4H6BrF3/c5-3-1-2-4(6,7)8/h1-3H2
**InchiKey:** DBCAQXHNJOFNGC-UHFFFAOYSA-N
**Formula:** C4H6BrF3
**SMILES:** FC(F)(F)CCCBr
**Mol. weight [g/mol]:** 190.99
**CAS:** 406-81-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -584.47 | kJ/mol | Joback Method |
| hf | -696.64 | kJ/mol | Joback Method |
| hfus | 13.23 | kJ/mol | Joback Method |
| hvap | 27.19 | kJ/mol | Joback Method |
| log10ws | -2.59 | | Crippen Method |
| logp | 2.724 | | Crippen Method |
| mcvol | 90.030 | ml/mol | McGowan Method |
| pc | 3677.55 | kPa | Joback Method |
| tb | 351.66 | K | Joback Method |
| tc | 518.63 | K | Joback Method |
| tf | 198.83 | K | Joback Method |
| vc | 0.364 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 153.13 | J/mol×K | 351.66 | Joback Method |
| cpg | 161.24 | J/mol×K | 379.49 | Joback Method |
| cpg | 168.88 | J/mol×K | 407.32 | Joback Method |
| cpg | 176.07 | J/mol×K | 435.15 | Joback Method |
| cpg | 182.83 | J/mol×K | 462.98 | Joback Method |
| cpg | 189.18 | J/mol×K | 490.81 | Joback Method |
| cpg | 195.14 | J/mol×K | 518.63 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C406815&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

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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 |