# 1-Bromo-1,1,2,3,3,3-hexafluoropropane

**Inchi:** InChI=1S/C3HBrF6/c4-2(6,7)1(5)3(8,9)10/h1H
**InchiKey:** UBSZSCBAJXCXOO-UHFFFAOYSA-N
**Formula:** C3HBrF6
**SMILES:** FC(C(F)(F)F)C(F)(F)Br
**Mol. weight [g/mol]:** 230.93
**CAS:** 2252-78-0

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1176.92 | kJ/mol | Joback Method |
| hf | -1278.36 | kJ/mol | Joback Method |
| hfus | 8.94 | kJ/mol | Joback Method |
| hvap | 20.82 | kJ/mol | Joback Method |
| log10ws | -2.95 | | Crippen Method |
| logp | 2.875 | | Crippen Method |
| mcvol | 81.250 | ml/mol | McGowan Method |
| pc | 3624.61 | kPa | Joback Method |
| tb | 308.60 | K | NIST Webbook |
| tc | 476.41 | K | Joback Method |
| tf | 176.75 | K | Joback Method |
| vc | 0.345 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 145.40 | J/mol×K | 322.92 | Joback Method |
| cpg | 152.94 | J/mol×K | 348.50 | Joback Method |
| cpg | 159.93 | J/mol×K | 374.08 | Joback Method |
| cpg | 166.42 | J/mol×K | 399.66 | Joback Method |
| cpg | 172.42 | J/mol×K | 425.24 | Joback Method |
| cpg | 177.95 | J/mol×K | 450.82 | Joback Method |
| cpg | 183.03 | J/mol×K | 476.41 | 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=C2252780&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 |