# Benzene, (1-bromo-2,2,2-trifluoroethyl)

**Inchi:** InChI=1S/C8H6BrF3/c9-7(8(10,11)12)6-4-2-1-3-5-6/h1-5,7H
**InchiKey:** IRICHAOGAOFEQI-UHFFFAOYSA-N
**Formula:** C8H6BrF3
**SMILES:** FC(F)(F)C(Br)c1ccccc1
**Mol. weight [g/mol]:** 239.03

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -440.82 | kJ/mol | Joback Method |
| hf | -547.95 | kJ/mol | Joback Method |
| hfus | 14.10 | kJ/mol | Joback Method |
| hvap | 37.98 | kJ/mol | Joback Method |
| log10ws | -3.83 | | Crippen Method |
| logp | 3.685 | | Crippen Method |
| mcvol | 122.630 | ml/mol | McGowan Method |
| pc | 3484.76 | kPa | Joback Method |
| rinpol | 1030.00 | | NIST Webbook |
| rinpol | 1030.00 | | NIST Webbook |
| rinpol | 1023.00 | | NIST Webbook |
| tb | 469.42 | K | Joback Method |
| tc | 681.31 | K | Joback Method |
| tf | 255.33 | K | Joback Method |
| vc | 0.474 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 241.21 | J/mol×K | 469.42 | Joback Method |
| cpg | 253.08 | J/mol×K | 504.73 | Joback Method |
| cpg | 263.98 | J/mol×K | 540.05 | Joback Method |
| cpg | 273.98 | J/mol×K | 575.36 | Joback Method |
| cpg | 283.14 | J/mol×K | 610.68 | Joback Method |
| cpg | 291.51 | J/mol×K | 645.99 | Joback Method |
| cpg | 299.17 | J/mol×K | 681.31 | 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=R345314&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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |