# Benzene, 1-bromo-2,4-difluoro-

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|---|---|
| **Other names:** | 1-Bromo-2,4-difluorobenzene |
| | 2,4-Difluorobromobenzene |
| | 2,4-Difluoro-1-bromobenzene |
| **Inchi:** | InChI=1S/C6H3BrF2/c7-5-2-1-4(8)3-6(5)9/h1-3H |
| **InchiKey:** | MGHBDQZXPCTTIH-UHFFFAOYSA-N |
| **Formula:** | C6H3BrF2 |
| **SMILES:** | Fc1ccc(Br)c(F)c1 |
| **Mol. weight [g/mol]:** | 192.99 |
| **CAS:** | 348-57-2 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -282.51 | kJ/mol | Joback Method |
| hf | -319.47 | kJ/mol | Joback Method |
| hfus | 16.00 | kJ/mol | Joback Method |
| hvap | 37.35 | kJ/mol | Joback Method |
| log10ws | -3.30 | | Crippen Method |
| logp | 2.727 | | Crippen Method |
| mcvol | 92.680 | ml/mol | McGowan Method |
| pc | 4362.63 | kPa | Joback Method |
| tb | 438.02 | K | Joback Method |
| tc | 651.05 | K | Joback Method |
| tf | 269.82 | K | Joback Method |
| vc | 0.361 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 152.73 | J/mol×K | 438.02 | Joback Method |
| cpg | 160.24 | J/mol×K | 473.53 | Joback Method |
| cpg | 167.26 | J/mol×K | 509.03 | Joback Method |
| cpg | 173.84 | J/mol×K | 544.54 | Joback Method |
| cpg | 179.98 | J/mol×K | 580.04 | Joback Method |
| cpg | 185.71 | J/mol×K | 615.55 | Joback Method |

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|---|---|---|---|---|
| cpg | 191.05 | J/mol×K | 651.05 | 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=C348572&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 |