# Benzoic acid, 4-bromo-, methyl ester

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|---|---|
| **Other names:** | 4-Bromobenzoic acid, methyl ester |
| | Benzoic acid, p-bromo-, methyl ester |
| | methyl 4-bromobenzoate |
| | methyl p-bromobenzoate |
| | p-Bromobenzoic acid, methyl ester |
| **Inchi:** | InChI=1S/C8H7BrO2/c1-11-8(10)6-2-4-7(9)5-3-6/h2-5H,1H3 |
| **InchiKey:** | CZNGTXVOZOWWKM-UHFFFAOYSA-N |
| **Formula:** | C8H7BrO2 |
| **SMILES:** | COC(=O)c1ccc(Br)cc1 |
| **Mol. weight [g/mol]:** | 215.04 |
| **CAS:** | 619-42-1 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -100.34 | kJ/mol | Joback Method |
| hf | -201.86 | kJ/mol | Joback Method |
| hfus | 18.20 | kJ/mol | Joback Method |
| hvap | 51.93 | kJ/mol | Joback Method |
| ie | 9.47 | eV | NIST Webbook |
| log10ws | -2.88 | | Crippen Method |
| logp | 2.236 | | Crippen Method |
| mcvol | 124.760 | ml/mol | McGowan Method |
| pc | 4135.61 | kPa | Joback Method |
| rinpol | 1336.00 | | NIST Webbook |
| rinpol | 1336.00 | | NIST Webbook |
| rinpol | 1336.00 | | NIST Webbook |
| tb | 556.55 | K | Joback Method |
| tc | 792.86 | K | Joback Method |
| tf | 351.22 | K | The influence of the halogen size in the volatility and melting of methyl p-halobenzoic esters and of their parent acids |
| vc | 0.462 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 246.83 | J/mol×K | 556.55 | Joback Method |
| cpg | 257.12 | J/mol×K | 595.93 | Joback Method |
| cpg | 266.74 | J/mol×K | 635.32 | Joback Method |
| cpg | 275.70 | J/mol×K | 674.70 | Joback Method |
| cpg | 284.02 | J/mol×K | 714.09 | Joback Method |
| cpg | 291.72 | J/mol×K | 753.47 | Joback Method |
| cpg | 298.81 | J/mol×K | 792.86 | Joback Method |
| dvisc | 0.0015564 | Pa×s | 350.82 | Joback Method |
| dvisc | 0.0010113 | Pa×s | 385.11 | Joback Method |
| dvisc | 0.0007051 | Pa×s | 419.40 | Joback Method |
| dvisc | 0.0005191 | Pa×s | 453.69 | Joback Method |
| dvisc | 0.0003990 | Pa×s | 487.97 | Joback Method |
| dvisc | 0.0003175 | Pa×s | 522.26 | Joback Method |
| dvisc | 0.0002598 | Pa×s | 556.55 | Joback Method |

# Sources

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|---|---|
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **The influence of the halogen size in the volatility and melting of methyl p-halobenzoic esters and of their parent acids:** | https://www.doi.org/10.1016/j.jct.2012.07.027 |
| **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=C619421&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **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 |
| **ie:** | Ionization energy |

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|---|---|
| **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 |