# Benzoic acid 2-bromoethyl ester

**Other names:** 2-Bromoethyl benzoate
**Inchi:** InChI=1S/C9H9BrO2/c10-6-7-12-9(11)8-4-2-1-3-5-8/h1-5H,6-7H2
**InchiKey:** KNBBDZULQFKSIE-UHFFFAOYSA-N
**Formula:** C9H9BrO2
**SMILES:** O=C(OCCBr)c1ccccc1
**Mol. weight [g/mol]:** 229.07
**CAS:** 939-54-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -82.29 | kJ/mol | Joback Method |
| hf | -211.03 | kJ/mol | Joback Method |
| hfus | 21.18 | kJ/mol | Joback Method |
| hvap | 53.50 | kJ/mol | Joback Method |
| log10ws | -2.56 | | Crippen Method |
| logp | 2.238 | | Crippen Method |
| mcvol | 138.850 | ml/mol | McGowan Method |
| pc | 3736.23 | kPa | Joback Method |
| tb | 574.45 | K | Joback Method |
| tc | 805.03 | K | Joback Method |
| tf | 349.57 | K | Joback Method |
| vc | 0.517 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 292.03 | J/mol×K | 574.45 | Joback Method |
| cpg | 303.67 | J/mol×K | 612.88 | Joback Method |
| cpg | 314.52 | J/mol×K | 651.31 | Joback Method |
| cpg | 324.59 | J/mol×K | 689.74 | Joback Method |
| cpg | 333.94 | J/mol×K | 728.17 | Joback Method |
| cpg | 342.57 | J/mol×K | 766.60 | Joback Method |
| cpg | 350.54 | J/mol×K | 805.03 | Joback Method |
| dvisc | 0.0019077 | Pa×s | 349.57 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0011445 | Pa×s | 387.05 | Joback Method |
| dvisc | 0.0007515 | Pa×s | 424.53 | Joback Method |
| dvisc | 0.0005283 | Pa×s | 462.01 | Joback Method |
| dvisc | 0.0003915 | Pa×s | 499.49 | Joback Method |
| dvisc | 0.0003026 | Pa×s | 536.97 | Joback Method |
| dvisc | 0.0002418 | Pa×s | 574.45 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C939548&Units=SI |

# Legend

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