# METHYL 3,5-DIBROMOBENZOATE

**Other names:** Benzoic acid, 3,5-dibromo-, methyl ester
**Inchi:** InChI=1S/C8H6Br2O2/c1-12-8(11)5-2-6(9)4-7(10)3-5/h2-4H,1H3
**InchiKey:** GSMAWUZTAIOCPL-UHFFFAOYSA-N
**Formula:** C8H6Br2O2
**SMILES:** COC(=O)c1cc(Br)cc(Br)c1
**Mol. weight [g/mol]:** 293.94

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.5274 | | Cheméo Relay (1.0) |
| hf | -245.20 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 23.10 | kJ/mol | Joback Method |
| hvap | 76.45 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.28 | eV | Cheméo Relay (1.0) |
| log10ws | -4.44 | | Cheméo Relay (1.0) |
| logp | 2.998 | | Crippen Method |
| mcvol | 142.260 | ml/mol | McGowan Method |
| pc | 4438.52 | kPa | Joback Method |
| rinpol | 1614.00 | | NIST Webbook |
| tb | 556.27 | K | Cheméo Relay (1.0) |
| tc | 771.74 | K | Cheméo Relay (1.0) |
| tf | 368.45 | K | Cheméo Relay (1.0) |
| vc | 0.488 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 274.61 | J/mol×K | 627.69 | Joback Method |
| cpg | 283.58 | J/mol×K | 669.45 | Joback Method |
| cpg | 291.87 | J/mol×K | 711.20 | Joback Method |
| cpg | 299.53 | J/mol×K | 752.96 | Joback Method |
| cpg | 306.56 | J/mol×K | 794.71 | Joback Method |
| cpg | 313.01 | J/mol×K | 836.47 | Joback Method |
| cpg | 318.89 | J/mol×K | 878.22 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0010566 | Pa×s | 423.14 | Joback Method |
| dvisc | 0.0007517 | Pa×s | 457.23 | Joback Method |
| dvisc | 0.0005606 | Pa×s | 491.32 | Joback Method |
| dvisc | 0.0004344 | Pa×s | 525.42 | Joback Method |
| dvisc | 0.0003472 | Pa×s | 559.51 | Joback Method |
| dvisc | 0.0002847 | Pa×s | 593.60 | Joback Method |
| dvisc | 0.0002385 | Pa×s | 627.69 | Joback Method |

# Sources

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|---|---|
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C51329158&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

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|---|---|
| **af:** | Acentric Factor |
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **ie:** | Ionization energy |
| **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 |