# Propanoic acid, 3-bromo-, methyl ester

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|---|---|
| **Other names:** | Propionic acid, 3-bromo-, methyl ester |
| | «beta»-Bromopropionic acid, methyl ester |
| | Methyl «beta»-bromopropionate |
| | Methyl 3-bromopropanoate |
| | Methyl 3-bromopropionate |
| | 3-Bromopropionic acid methyl ester |
| **Inchi:** | InChI=1S/C4H7BrO2/c1-7-4(6)2-3-5/h2-3H2,1H3 |
| **InchiKey:** | KQEVIFKPZOGBMZ-UHFFFAOYSA-N |
| **Formula:** | C4H7BrO2 |
| **SMILES:** | COC(=O)CCBr |
| **Mol. weight [g/mol]:** | 167.00 |
| **CAS:** | 3395-91-3 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -236.80 | kJ/mol | Joback Method |
| hf | -344.36 | kJ/mol | Joback Method |
| hfus | 14.19 | kJ/mol | Joback Method |
| hvap | 40.09 | kJ/mol | Joback Method |
| log10ws | -0.79 | | Crippen Method |
| logp | 0.944 | | Crippen Method |
| mcvol | 92.160 | ml/mol | McGowan Method |
| pc | 4522.49 | kPa | Joback Method |
| rinpol | 902.00 | | NIST Webbook |
| tb | 433.37 | K | Joback Method |
| tc | 632.29 | K | Joback Method |
| tf | 266.80 | K | Joback Method |
| vc | 0.345 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 158.76 | J/mol×K | 433.37 | Joback Method |
| cpg | 165.82 | J/mol×K | 466.52 | Joback Method |

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|---|---|---|---|---|
| cpg | 172.60 | J/mol×K | 499.68 | Joback Method |
| cpg | 179.11 | J/mol×K | 532.83 | Joback Method |
| cpg | 185.34 | J/mol×K | 565.98 | Joback Method |
| cpg | 191.30 | J/mol×K | 599.13 | Joback Method |
| cpg | 196.99 | J/mol×K | 632.29 | Joback Method |
| dvisc | 0.0026007 | Pa×s | 266.80 | Joback Method |
| dvisc | 0.0016199 | Pa×s | 294.56 | Joback Method |
| dvisc | 0.0010947 | Pa×s | 322.32 | Joback Method |
| dvisc | 0.0007873 | Pa×s | 350.09 | Joback Method |
| dvisc | 0.0005942 | Pa×s | 377.85 | Joback Method |
| dvisc | 0.0004662 | Pa×s | 405.61 | Joback Method |
| dvisc | 0.0003772 | Pa×s | 433.37 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C3395913&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |