# Isobutyl 3-bromopropanoate

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|---|---|
| **Other names:** | Propanoic acid, 3-bromo, isobutyl ester |
| **Inchi:** | InChI=1S/C7H13BrO2/c1-6(2)5-10-7(9)3-4-8/h6H,3-5H2,1-2H3 |
| **InchiKey:** | SMOUSNHACQMSQG-UHFFFAOYSA-N |
| **Formula:** | C7H13BrO2 |
| **SMILES:** | CC(C)COC(=O)CCBr |
| **Mol. weight [g/mol]:** | 209.08 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -213.98 | kJ/mol | Joback Method |
| hf | -411.56 | kJ/mol | Joback Method |
| hfus | 18.43 | kJ/mol | Joback Method |
| hvap | 46.38 | kJ/mol | Joback Method |
| log10ws | -1.81 | | Crippen Method |
| logp | 1.971 | | Crippen Method |
| mcvol | 134.430 | ml/mol | McGowan Method |
| pc | 3202.78 | kPa | Joback Method |
| rinpol | 1136.00 | | NIST Webbook |
| ripol | 1586.00 | | NIST Webbook |
| ripol | 1586.00 | | NIST Webbook |
| tb | 501.57 | K | Joback Method |
| tc | 697.81 | K | Joback Method |
| tf | 285.61 | K | Joback Method |
| vc | 0.507 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 277.07 | J/mol×K | 501.57 | Joback Method |
| cpg | 288.28 | J/mol×K | 534.28 | Joback Method |
| cpg | 298.99 | J/mol×K | 566.98 | Joback Method |
| cpg | 309.20 | J/mol×K | 599.69 | Joback Method |
| cpg | 318.93 | J/mol×K | 632.40 | Joback Method |
| cpg | 328.18 | J/mol×K | 665.11 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 336.97 | J/mol×K | 697.81 | Joback Method |
| dvisc | 0.0034561 | Pa×s | 285.61 | Joback Method |
| dvisc | 0.0018031 | Pa×s | 321.60 | Joback Method |
| dvisc | 0.0010723 | Pa×s | 357.60 | Joback Method |
| dvisc | 0.0007013 | Pa×s | 393.59 | Joback Method |
| dvisc | 0.0004925 | Pa×s | 429.58 | Joback Method |
| dvisc | 0.0003653 | Pa×s | 465.58 | Joback Method |
| dvisc | 0.0002828 | Pa×s | 501.57 | Joback Method |

# Sources

**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=R30143&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
**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
**ripol:** Polar retention indices
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point
**vc:** Critical Volume

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