# 3-(4-Bromobenzoyl)propionic acid

**Other names:** 3-(p-Bromobenzoyl)propionic acid
«beta»-(p-Bromobenzoyl)propionic acid
Benzenebutanoic acid, 4-bromo-«gamma»-oxo-
**Inchi:** InChI=1S/C10H9BrO3/c11-8-3-1-7(2-4-8)9(12)5-6-10(13)14/h1-4H,5-6H2,(H,13,14)
**InchiKey:** ZODFRCZNTXLDDW-UHFFFAOYSA-N
**Formula:** C10H9BrO3
**SMILES:** O=C(O)CCC(=O)c1ccc(Br)cc1
**Mol. weight [g/mol]:** 257.08
**CAS:** 6340-79-0

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -244.24 | kJ/mol | Joback Method |
| hf | -375.73 | kJ/mol | Joback Method |
| hfus | 27.88 | kJ/mol | Joback Method |
| hvap | 77.40 | kJ/mol | Joback Method |
| log10ws | -3.23 | | Crippen Method |
| logp | 2.497 | | Crippen Method |
| mcvol | 154.510 | ml/mol | McGowan Method |
| pc | 4031.24 | kPa | Joback Method |
| tb | 725.94 | K | Joback Method |
| tc | 944.68 | K | Joback Method |
| tf | 461.88 | K | Joback Method |
| vc | 0.581 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 368.24 | J/mol×K | 725.94 | Joback Method |
| cpg | 376.91 | J/mol×K | 762.40 | Joback Method |
| cpg | 384.94 | J/mol×K | 798.85 | Joback Method |
| cpg | 392.37 | J/mol×K | 835.31 | Joback Method |
| cpg | 399.23 | J/mol×K | 871.77 | Joback Method |
| cpg | 405.57 | J/mol×K | 908.22 | Joback Method |

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|---|---|---|---|---|
| cpg | 411.42 | J/mol×K | 944.68 | Joback Method |
| dvisc | 0.0011687 | Pa×s | 461.88 | Joback Method |
| dvisc | 0.0005788 | Pa×s | 505.89 | Joback Method |
| dvisc | 0.0003208 | Pa×s | 549.90 | Joback Method |
| dvisc | 0.0001940 | Pa×s | 593.91 | Joback Method |
| dvisc | 0.0001258 | Pa×s | 637.92 | Joback Method |
| dvisc | 0.0000862 | Pa×s | 681.93 | Joback Method |
| dvisc | 0.0000619 | Pa×s | 725.94 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C6340790&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

**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