# Phthalic acid, 2-(3-bromophenyl)ethyl isobutyl ester

**Inchi:** InChI=1S/C20H21BrO4/c1-14(2)13-25-20(23)18-9-4-3-8-17(18)19(22)24-11-10-15-6-5-7-

**InchiKey:** ARALGHDGXPQMMM-UHFFFAOYSA-N

**Formula:** C20H21BrO4

**SMILES:** CC(C)COC(=O)c1ccccc1C(=O)OCCc1cccc(Br)c1

**Mol. weight [g/mol]:** 405.28

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -132.88 | kJ/mol | Joback Method |
| hf | -474.56 | kJ/mol | Joback Method |
| hfus | 42.20 | kJ/mol | Joback Method |
| hvap | 90.35 | kJ/mol | Joback Method |
| log10ws | -6.17 | | Crippen Method |
| logp | 4.661 | | Crippen Method |
| mcvol | 277.520 | ml/mol | McGowan Method |
| pc | 1830.98 | kPa | Joback Method |
| rinpol | 2738.00 | | NIST Webbook |
| tb | 938.62 | K | Joback Method |
| tc | 1175.56 | K | Joback Method |
| tf | 582.16 | K | Joback Method |
| vc | 1.044 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 814.22 | J/mol×K | 938.62 | Joback Method |
| cpg | 826.45 | J/mol×K | 978.11 | Joback Method |
| cpg | 837.38 | J/mol×K | 1017.60 | Joback Method |
| cpg | 847.07 | J/mol×K | 1057.09 | Joback Method |
| cpg | 855.56 | J/mol×K | 1096.58 | Joback Method |
| cpg | 862.91 | J/mol×K | 1136.07 | Joback Method |
| cpg | 869.16 | J/mol×K | 1175.56 | Joback Method |
| dvisc | 0.0003364 | Pa×s | 582.16 | Joback Method |
| dvisc | 0.0002017 | Pa×s | 641.57 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001318 | Pa×s | 700.98 | Joback Method |
| dvisc | 0.0000921 | Pa×s | 760.39 | Joback Method |
| dvisc | 0.0000678 | Pa×s | 819.80 | Joback Method |
| dvisc | 0.0000520 | Pa×s | 879.21 | Joback Method |
| dvisc | 0.0000412 | Pa×s | 938.62 | Joback Method |

# Sources

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|---|---|
| **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=U378022&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |