# Isophthalic acid, 4-bromophenyl ethyl ester

**Inchi:** InChI=1S/C16H13BrO4/c1-2-20-15(18)11-4-3-5-12(10-11)16(19)21-14-8-6-13(17)7-9-14/
**InchiKey:** HNCYHYNDUHJADC-UHFFFAOYSA-N
**Formula:** C16H13BrO4
**SMILES:** CCOC(=O)c1cccc(C(=O)Oc2ccc(Br)cc2)c1
**Mol. weight [g/mol]:** 349.18

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -164.12 | kJ/mol | Joback Method |
| hf | -386.72 | kJ/mol | Joback Method |
| hfus | 35.36 | kJ/mol | Joback Method |
| hvap | 81.83 | kJ/mol | Joback Method |
| log10ws | -5.38 | | Crippen Method |
| logp | 3.845 | | Crippen Method |
| mcvol | 221.160 | ml/mol | McGowan Method |
| pc | 2600.43 | kPa | Joback Method |
| rinpol | 2575.00 | | NIST Webbook |
| rinpol | 2575.00 | | NIST Webbook |
| tb | 847.54 | K | Joback Method |
| tc | 1093.22 | K | Joback Method |
| tf | 552.08 | K | Joback Method |
| vc | 0.826 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 588.98 | J/mol×K | 847.54 | Joback Method |
| cpg | 634.78 | J/mol×K | 1052.27 | Joback Method |
| cpg | 627.86 | J/mol×K | 1011.32 | Joback Method |
| cpg | 619.86 | J/mol×K | 970.38 | Joback Method |
| cpg | 610.74 | J/mol×K | 929.43 | Joback Method |
| cpg | 600.46 | J/mol×K | 888.49 | Joback Method |
| cpg | 640.65 | J/mol×K | 1093.22 | Joback Method |
| dvisc | 0.0000798 | Pa×s | 847.54 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000979 | Pa×s | 798.30 | Joback Method |
| dvisc | 0.0001233 | Pa×s | 749.05 | Joback Method |
| dvisc | 0.0001605 | Pa×s | 699.81 | Joback Method |
| dvisc | 0.0002173 | Pa×s | 650.57 | Joback Method |
| dvisc | 0.0003092 | Pa×s | 601.32 | Joback Method |
| dvisc | 0.0004686 | Pa×s | 552.08 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U344463&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 |