# Terephthalic acid, butyl 2-iodobenzyl ester

**Inchi:** InChI=1S/C19H19IO4/c1-2-3-12-23-18(21)14-8-10-15(11-9-14)19(22)24-13-16-6-4-5-7-1
**InchiKey:** MJFVTRGORZEIAY-UHFFFAOYSA-N
**Formula:** C19H19IO4
**SMILES:** CCCCOC(=O)c1ccc(C(=O)OCc2ccccc2I)cc1
**Mol. weight [g/mol]:** 438.26

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -95.06 | kJ/mol | Joback Method |
| hf | -398.10 | kJ/mol | Joback Method |
| hfus | 42.25 | kJ/mol | Joback Method |
| hvap | 91.45 | kJ/mol | Joback Method |
| log10ws | -6.47 | | Crippen Method |
| logp | 4.605 | | Crippen Method |
| mcvol | 271.750 | ml/mol | McGowan Method |
| pc | 1826.28 | kPa | Joback Method |
| rinpol | 3078.00 | | NIST Webbook |
| rinpol | 3078.00 | | NIST Webbook |
| tb | 943.16 | K | Joback Method |
| tc | 1189.04 | K | Joback Method |
| tf | 584.15 | K | Joback Method |
| vc | 1.020 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 765.00 | J/mol×K | 943.16 | Joback Method |
| cpg | 776.52 | J/mol×K | 984.14 | Joback Method |
| cpg | 786.76 | J/mol×K | 1025.12 | Joback Method |
| cpg | 795.78 | J/mol×K | 1066.10 | Joback Method |
| cpg | 803.62 | J/mol×K | 1107.08 | Joback Method |
| cpg | 810.34 | J/mol×K | 1148.06 | Joback Method |
| cpg | 815.99 | J/mol×K | 1189.04 | Joback Method |
| dvisc | 0.0003723 | Pa×s | 584.15 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002254 | Pa×s | 643.99 | Joback Method |
| dvisc | 0.0001486 | Pa×s | 703.82 | Joback Method |
| dvisc | 0.0001046 | Pa×s | 763.65 | Joback Method |
| dvisc | 0.0000774 | Pa×s | 823.49 | Joback Method |
| dvisc | 0.0000597 | Pa×s | 883.33 | Joback Method |
| dvisc | 0.0000476 | Pa×s | 943.16 | 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=U416073&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 |