# Terephthalic acid, 4-bromobenzyl pentyl ester

**Inchi:** InChI=1S/C20H21BrO4/c1-2-3-4-13-24-19(22)16-7-9-17(10-8-16)20(23)25-14-15-5-11-18
**InchiKey:** BBVKXQGVCBDTLU-UHFFFAOYSA-N
**Formula:** C20H21BrO4
**SMILES:** CCCCCOC(=O)c1ccc(C(=O)OCc2ccc(Br)cc2)cc1
**Mol. weight [g/mol]:** 405.28

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -130.44 | kJ/mol | Joback Method |
| hf | -469.28 | kJ/mol | Joback Method |
| hfus | 45.72 | kJ/mol | Joback Method |
| hvap | 90.74 | kJ/mol | Joback Method |
| log10ws | -6.90 | | Crippen Method |
| logp | 5.153 | | Crippen Method |
| mcvol | 277.520 | ml/mol | McGowan Method |
| pc | 1818.50 | kPa | Joback Method |
| rinpol | 3184.00 | | NIST Webbook |
| rinpol | 3184.00 | | NIST Webbook |
| tb | 939.06 | K | Joback Method |
| tc | 1173.28 | K | Joback Method |
| tf | 597.16 | K | Joback Method |
| vc | 1.050 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 813.72 | J/mol×K | 939.06 | Joback Method |
| cpg | 862.41 | J/mol×K | 1134.24 | Joback Method |
| cpg | 854.98 | J/mol×K | 1095.21 | Joback Method |
| cpg | 846.44 | J/mol×K | 1056.17 | Joback Method |
| cpg | 836.75 | J/mol×K | 1017.13 | Joback Method |
| cpg | 825.86 | J/mol×K | 978.10 | Joback Method |
| cpg | 868.78 | J/mol×K | 1173.28 | Joback Method |
| dvisc | 0.0000452 | Pa×s | 939.06 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000563 | Pa×s | 882.08 | Joback Method |
| dvisc | 0.0000722 | Pa×s | 825.09 | Joback Method |
| dvisc | 0.0000961 | Pa×s | 768.11 | Joback Method |
| dvisc | 0.0001339 | Pa×s | 711.13 | Joback Method |
| dvisc | 0.0001976 | Pa×s | 654.14 | Joback Method |
| dvisc | 0.0003142 | Pa×s | 597.16 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U415961&Units=SI |

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |