# Terephthalic acid, 2-bromobenzyl propyl ester

**Inchi:** InChI=1S/C18H17BrO4/c1-2-11-22-17(20)13-7-9-14(10-8-13)18(21)23-12-15-5-3-4-6-16(
**InchiKey:** HXIWMTGMOAZVQL-UHFFFAOYSA-N
**Formula:** C18H17BrO4
**SMILES:** CCCOC(=O)c1ccc(C(=O)OCc2ccccc2Br)cc1
**Mol. weight [g/mol]:** 377.23

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -147.28 | kJ/mol | Joback Method |
| hf | -428.00 | kJ/mol | Joback Method |
| hfus | 40.54 | kJ/mol | Joback Method |
| hvap | 86.28 | kJ/mol | Joback Method |
| log10ws | -6.07 | | Crippen Method |
| logp | 4.373 | | Crippen Method |
| mcvol | 249.340 | ml/mol | McGowan Method |
| pc | 2157.31 | kPa | Joback Method |
| rinpol | 2782.00 | | NIST Webbook |
| rinpol | 2782.00 | | NIST Webbook |
| tb | 893.30 | K | Joback Method |
| tc | 1131.83 | K | Joback Method |
| tf | 574.62 | K | Joback Method |
| vc | 0.938 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 699.78 | J/mol×K | 893.30 | Joback Method |
| cpg | 711.67 | J/mol×K | 933.06 | Joback Method |
| cpg | 722.33 | J/mol×K | 972.81 | Joback Method |
| cpg | 731.82 | J/mol×K | 1012.57 | Joback Method |
| cpg | 740.17 | J/mol×K | 1052.32 | Joback Method |
| cpg | 747.42 | J/mol×K | 1092.08 | Joback Method |
| cpg | 753.62 | J/mol×K | 1131.83 | Joback Method |
| dvisc | 0.0003867 | Pa×s | 574.62 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0002489 | Pa×s | 627.73 | Joback Method |
| dvisc | 0.0001716 | Pa×s | 680.85 | Joback Method |
| dvisc | 0.0001249 | Pa×s | 733.96 | Joback Method |
| dvisc | 0.0000949 | Pa×s | 787.07 | Joback Method |
| dvisc | 0.0000746 | Pa×s | 840.19 | Joback Method |
| dvisc | 0.0000604 | Pa×s | 893.30 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U416078&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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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