# 1,2-Propanediol, dibenzoate

**Other names:** propane-1,2-diyl dibenzoate
**Inchi:** InChI=1S/C17H16O4/c1-13(21-17(19)15-10-6-3-7-11-15)12-20-16(18)14-8-4-2-5-9-14/h2
**InchiKey:** UMVMVEZHMZTUHD-UHFFFAOYSA-N
**Formula:** C17H16O4
**SMILES:** CC(COC(=O)c1ccccc1)OC(=O)c1ccccc1
**Mol. weight [g/mol]:** 284.31
**CAS:** 19224-26-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -153.20 | kJ/mol | Joback Method |
| hf | -416.03 | kJ/mol | Joback Method |
| hfus | 29.92 | kJ/mol | Joback Method |
| hvap | 75.91 | kJ/mol | Joback Method |
| log10ws | -4.14 | | Crippen Method |
| logp | 3.089 | | Crippen Method |
| mcvol | 217.750 | ml/mol | McGowan Method |
| pc | 2293.71 | kPa | Joback Method |
| tb | 793.86 | K | Joback Method |
| tc | 1029.01 | K | Joback Method |
| tf | 463.51 | K | Joback Method |
| vc | 0.814 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 614.70 | J/mol×K | 793.86 | Joback Method |
| cpg | 628.81 | J/mol×K | 833.05 | Joback Method |
| cpg | 641.63 | J/mol×K | 872.24 | Joback Method |
| cpg | 653.19 | J/mol×K | 911.43 | Joback Method |
| cpg | 663.54 | J/mol×K | 950.63 | Joback Method |
| cpg | 672.71 | J/mol×K | 989.82 | Joback Method |
| cpg | 680.74 | J/mol×K | 1029.01 | Joback Method |
| dvisc | 0.0009003 | Pa×s | 463.51 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0004793 | Pa×s | 518.57 | Joback Method |
| dvisc | 0.0002880 | Pa×s | 573.63 | Joback Method |
| dvisc | 0.0001892 | Pa×s | 628.69 | Joback Method |
| dvisc | 0.0001330 | Pa×s | 683.74 | Joback Method |
| dvisc | 0.0000985 | Pa×s | 738.80 | Joback Method |
| dvisc | 0.0000761 | Pa×s | 793.86 | 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=C19224261&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |