# Diglycolic acid, butyl 2-isopropylphenyl ester

**Inchi:** InChI=1S/C17H24O5/c1-4-5-10-21-16(18)11-20-12-17(19)22-15-9-7-6-8-14(15)13(2)3/h6
**InchiKey:** XQAFHZNVEBXBAN-UHFFFAOYSA-N
**Formula:** C17H24O5
**SMILES:** CCCCOC(=O)COCC(=O)Oc1ccccc1C(C)C
**Mol. weight [g/mol]:** 308.37

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -380.24 | kJ/mol | Joback Method |
| hf | -796.25 | kJ/mol | Joback Method |
| hfus | 36.68 | kJ/mol | Joback Method |
| hvap | 76.71 | kJ/mol | Joback Method |
| log10ws | -3.43 | | Crippen Method |
| logp | 3.075 | | Crippen Method |
| mcvol | 247.380 | ml/mol | McGowan Method |
| pc | 1664.61 | kPa | Joback Method |
| rinpol | 2572.00 | | NIST Webbook |
| rinpol | 2572.00 | | NIST Webbook |
| tb | 794.58 | K | Joback Method |
| tc | 997.23 | K | Joback Method |
| tf | 471.84 | K | Joback Method |
| vc | 0.940 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 733.23 | J/mol×K | 794.58 | Joback Method |
| cpg | 748.43 | J/mol×K | 828.36 | Joback Method |
| cpg | 762.53 | J/mol×K | 862.13 | Joback Method |
| cpg | 775.55 | J/mol×K | 895.91 | Joback Method |
| cpg | 787.49 | J/mol×K | 929.68 | Joback Method |
| cpg | 798.35 | J/mol×K | 963.46 | Joback Method |
| cpg | 808.13 | J/mol×K | 997.23 | Joback Method |
| dvisc | 0.0006330 | Pa×s | 471.84 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0003456 | Pa×s | 525.63 | Joback Method |
| dvisc | 0.0002112 | Pa×s | 579.42 | Joback Method |
| dvisc | 0.0001403 | Pa×s | 633.21 | Joback Method |
| dvisc | 0.0000994 | Pa×s | 687.00 | Joback Method |
| dvisc | 0.0000740 | Pa×s | 740.79 | Joback Method |
| dvisc | 0.0000573 | Pa×s | 794.58 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U382288&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 |

# 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 |