# Diglycolic acid, di(2-acetylphenyl) ester

**Inchi:** InChI=1S/C20H18O7/c1-13(21)15-7-3-5-9-17(15)26-19(23)11-25-12-20(24)27-18-10-6-4
**InchiKey:** VVMWPLAKJAFVAP-UHFFFAOYSA-N
**Formula:** C20H18O7
**SMILES:** CC(=O)c1ccccc1OC(=O)COCC(=O)Oc1ccccc1C(C)=O
**Mol. weight [g/mol]:** 370.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -507.60 | kJ/mol | Joback Method |
| hf | -852.99 | kJ/mol | Joback Method |
| hfus | 44.82 | kJ/mol | Joback Method |
| hvap | 100.20 | kJ/mol | Joback Method |
| log10ws | -4.16 | | Crippen Method |
| logp | 2.619 | | Crippen Method |
| mcvol | 269.030 | ml/mol | McGowan Method |
| pc | 1882.17 | kPa | Joback Method |
| rinpol | 3205.00 | | NIST Webbook |
| rinpol | 3205.00 | | NIST Webbook |
| tb | 1003.06 | K | Joback Method |
| tc | 1240.69 | K | Joback Method |
| tf | 659.45 | K | Joback Method |
| vc | 1.018 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 820.32 | J/mol×K | 1003.06 | Joback Method |
| cpg | 847.42 | J/mol×K | 1201.08 | Joback Method |
| cpg | 845.09 | J/mol×K | 1161.48 | Joback Method |
| cpg | 841.22 | J/mol×K | 1121.87 | Joback Method |
| cpg | 835.81 | J/mol×K | 1082.27 | Joback Method |
| cpg | 828.85 | J/mol×K | 1042.66 | Joback Method |
| cpg | 848.23 | J/mol×K | 1240.69 | Joback Method |
| dvisc | 0.0000390 | Pa×s | 1003.06 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000482 | Pa×s | 945.79 | Joback Method |
| dvisc | 0.0000613 | Pa×s | 888.52 | Joback Method |
| dvisc | 0.0000804 | Pa×s | 831.25 | Joback Method |
| dvisc | 0.0001099 | Pa×s | 773.99 | Joback Method |
| dvisc | 0.0001579 | Pa×s | 716.72 | Joback Method |
| dvisc | 0.0002415 | Pa×s | 659.45 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U382730&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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