# Diglycolic acid, decyl 3-phenylpropyl ester

**Inchi:** InChI=1S/C23H36O5/c1-2-3-4-5-6-7-8-12-17-27-22(24)19-26-20-23(25)28-18-13-16-21-1
**InchiKey:** NEYYLXNLENETQA-UHFFFAOYSA-N
**Formula:** C23H36O5
**SMILES:** CCCCCCCCCCOC(=O)COCC(=O)OCCCc1ccccc1
**Mol. weight [g/mol]:** 392.53

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -317.65 | kJ/mol | Joback Method |
| hf | -903.34 | kJ/mol | Joback Method |
| hfus | 56.13 | kJ/mol | Joback Method |
| hvap | 89.79 | kJ/mol | Joback Method |
| log10ws | -5.37 | | Crippen Method |
| logp | 4.863 | | Crippen Method |
| mcvol | 331.920 | ml/mol | McGowan Method |
| pc | 1096.44 | kPa | Joback Method |
| rinpol | 3628.00 | | NIST Webbook |
| rinpol | 3628.00 | | NIST Webbook |
| tb | 927.32 | K | Joback Method |
| tc | 1135.98 | K | Joback Method |
| tf | 541.94 | K | Joback Method |
| vc | 1.282 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1088.48 | J/mol×K | 927.32 | Joback Method |
| cpg | 1104.78 | J/mol×K | 962.10 | Joback Method |
| cpg | 1119.66 | J/mol×K | 996.87 | Joback Method |
| cpg | 1133.17 | J/mol×K | 1031.65 | Joback Method |
| cpg | 1145.31 | J/mol×K | 1066.43 | Joback Method |
| cpg | 1156.12 | J/mol×K | 1101.20 | Joback Method |
| cpg | 1165.63 | J/mol×K | 1135.98 | Joback Method |
| dvisc | 0.0003438 | Pa×s | 541.94 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001780 | Pa×s | 606.17 | Joback Method |
| dvisc | 0.0001045 | Pa×s | 670.40 | Joback Method |
| dvisc | 0.0000674 | Pa×s | 734.63 | Joback Method |
| dvisc | 0.0000466 | Pa×s | 798.86 | Joback Method |
| dvisc | 0.0000340 | Pa×s | 863.09 | Joback Method |
| dvisc | 0.0000260 | Pa×s | 927.32 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U382179&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

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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 |