# Diglycolic acid, 2,5-dimethylphenyl propyl ester

**Inchi:** InChI=1S/C15H20O5/c1-4-7-19-14(16)9-18-10-15(17)20-13-8-11(2)5-6-12(13)3/h5-6,8H,

**InchiKey:** CNFKSNLOLXJXGF-UHFFFAOYSA-N

**Formula:** C15H20O5

**SMILES:** CCCOC(=O)COCC(=O)Oc1cc(C)ccc1C

**Mol. weight [g/mol]:** 280.32

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -404.27 | kJ/mol | Joback Method |
| hf | -761.16 | kJ/mol | Joback Method |
| hfus | 34.63 | kJ/mol | Joback Method |
| hvap | 73.31 | kJ/mol | Joback Method |
| log10ws | -2.78 | | Crippen Method |
| logp | 2.179 | | Crippen Method |
| mcvol | 219.200 | ml/mol | McGowan Method |
| pc | 1920.30 | kPa | Joback Method |
| rinpol | 2456.00 | | NIST Webbook |
| rinpol | 2456.00 | | NIST Webbook |
| tb | 754.24 | K | Joback Method |
| tc | 957.56 | K | Joback Method |
| tf | 476.82 | K | Joback Method |
| vc | 0.834 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 620.00 | J/mol×K | 754.24 | Joback Method |
| cpg | 682.11 | J/mol×K | 923.67 | Joback Method |
| cpg | 671.62 | J/mol×K | 889.79 | Joback Method |
| cpg | 660.15 | J/mol×K | 855.90 | Joback Method |
| cpg | 647.72 | J/mol×K | 822.01 | Joback Method |
| cpg | 634.33 | J/mol×K | 788.13 | Joback Method |
| cpg | 691.62 | J/mol×K | 957.56 | Joback Method |
| dvisc | 0.0000814 | Pa×s | 754.24 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001012 | Pa×s | 708.00 | Joback Method |
| dvisc | 0.0001297 | Pa×s | 661.77 | Joback Method |
| dvisc | 0.0001725 | Pa×s | 615.53 | Joback Method |
| dvisc | 0.0002402 | Pa×s | 569.29 | Joback Method |
| dvisc | 0.0003549 | Pa×s | 523.06 | Joback Method |
| dvisc | 0.0005654 | Pa×s | 476.82 | 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=U382704&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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |