# Diglycolic acid, 2-acetylphenyl hexyl ester

**Inchi:** InChI=1S/C18H24O6/c1-3-4-5-8-11-23-17(20)12-22-13-18(21)24-16-10-7-6-9-15(16)14(2
**InchiKey:** IVUFZHQECWBYKG-UHFFFAOYSA-N
**Formula:** C18H24O6
**SMILES:** CCCCCCOC(=O)COCC(=O)Oc1ccccc1C(C)=O
**Mol. weight [g/mol]:** 336.38

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -498.30 | kJ/mol | Joback Method |
| hf | -924.19 | kJ/mol | Joback Method |
| hfus | 44.39 | kJ/mol | Joback Method |
| hvap | 86.07 | kJ/mol | Joback Method |
| log10ws | -3.74 | | Crippen Method |
| logp | 2.935 | | Crippen Method |
| mcvol | 263.040 | ml/mol | McGowan Method |
| pc | 1610.29 | kPa | Joback Method |
| rinpol | 2973.00 | | NIST Webbook |
| rinpol | 2973.00 | | NIST Webbook |
| tb | 871.77 | K | Joback Method |
| tc | 1079.52 | K | Joback Method |
| tf | 548.04 | K | Joback Method |
| vc | 1.008 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 805.26 | J/mol×K | 871.77 | Joback Method |
| cpg | 818.67 | J/mol×K | 906.40 | Joback Method |
| cpg | 830.89 | J/mol×K | 941.02 | Joback Method |
| cpg | 841.91 | J/mol×K | 975.65 | Joback Method |
| cpg | 851.75 | J/mol×K | 1010.27 | Joback Method |
| cpg | 860.41 | J/mol×K | 1044.90 | Joback Method |
| cpg | 867.88 | J/mol×K | 1079.52 | Joback Method |
| dvisc | 0.0004247 | Pa×s | 548.04 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002561 | Pa×s | 602.00 | Joback Method |
| dvisc | 0.0001678 | Pa×s | 655.95 | Joback Method |
| dvisc | 0.0001173 | Pa×s | 709.90 | Joback Method |
| dvisc | 0.0000862 | Pa×s | 763.86 | Joback Method |
| dvisc | 0.0000660 | Pa×s | 817.82 | Joback Method |
| dvisc | 0.0000522 | Pa×s | 871.77 | Joback Method |

# Sources

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|---|---|
| **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=U382722&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |