# Diglycolic acid, di(2-methylpentyl) ester

**Inchi:** InChI=1S/C16H30O5/c1-5-7-13(3)9-20-15(17)11-19-12-16(18)21-10-14(4)8-6-2/h13-14H
**InchiKey:** HCEGVRQMNHKFAQ-UHFFFAOYSA-N
**Formula:** C16H30O5
**SMILES:** CCCC(C)COC(=O)COCC(=O)OCC(C)CCC
**Mol. weight [g/mol]:** 302.41

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -493.88 | kJ/mol | Joback Method |
| hf | -1005.95 | kJ/mol | Joback Method |
| hfus | 36.91 | kJ/mol | Joback Method |
| hvap | 71.16 | kJ/mol | Joback Method |
| log10ws | -2.85 | | Crippen Method |
| logp | 2.962 | | Crippen Method |
| mcvol | 257.050 | ml/mol | McGowan Method |
| pc | 1410.13 | kPa | Joback Method |
| rinpol | 2431.00 | | NIST Webbook |
| rinpol | 2431.00 | | NIST Webbook |
| tb | 739.60 | K | Joback Method |
| tc | 920.56 | K | Joback Method |
| tf | 406.63 | K | Joback Method |
| vc | 0.986 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 764.62 | J/mol×K | 739.60 | Joback Method |
| cpg | 781.34 | J/mol×K | 769.76 | Joback Method |
| cpg | 797.17 | J/mol×K | 799.92 | Joback Method |
| cpg | 812.09 | J/mol×K | 830.08 | Joback Method |
| cpg | 826.12 | J/mol×K | 860.24 | Joback Method |
| cpg | 839.25 | J/mol×K | 890.40 | Joback Method |
| cpg | 851.49 | J/mol×K | 920.56 | Joback Method |
| dvisc | 0.0012606 | Pa×s | 406.63 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0005594 | Pa×s | 462.12 | Joback Method |
| dvisc | 0.0002955 | Pa×s | 517.62 | Joback Method |
| dvisc | 0.0001766 | Pa×s | 573.12 | Joback Method |
| dvisc | 0.0001156 | Pa×s | 628.61 | Joback Method |
| dvisc | 0.0000810 | Pa×s | 684.11 | Joback Method |
| dvisc | 0.0000599 | Pa×s | 739.60 | 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=U381809&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 |