# Glutaric acid, 3-methylbenzyl pentyl ester

**Inchi:** InChI=1S/C18H26O4/c1-3-4-5-12-21-17(19)10-7-11-18(20)22-14-16-9-6-8-15(2)13-16/h6
**InchiKey:** LOMCSHATQNSABD-UHFFFAOYSA-N
**Formula:** C18H26O4
**SMILES:** CCCCCOC(=O)CCCC(=O)OCc1cccc(C)c1
**Mol. weight [g/mol]:** 306.40

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -264.38 | kJ/mol | Joback Method |
| hf | -679.39 | kJ/mol | Joback Method |
| hfus | 41.60 | kJ/mol | Joback Method |
| hvap | 76.91 | kJ/mol | Joback Method |
| log10ws | -4.74 | | Crippen Method |
| logp | 3.942 | | Crippen Method |
| mcvol | 255.600 | ml/mol | McGowan Method |
| pc | 1552.45 | kPa | Joback Method |
| rinpol | 2503.00 | | NIST Webbook |
| tb | 795.48 | K | Joback Method |
| tc | 995.15 | K | Joback Method |
| tf | 475.88 | K | Joback Method |
| vc | 0.984 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 761.25 | J/mol×K | 795.48 | Joback Method |
| cpg | 829.35 | J/mol×K | 961.87 | Joback Method |
| cpg | 817.75 | J/mol×K | 928.59 | Joback Method |
| cpg | 805.16 | J/mol×K | 895.32 | Joback Method |
| cpg | 791.55 | J/mol×K | 862.04 | Joback Method |
| cpg | 776.92 | J/mol×K | 828.76 | Joback Method |
| cpg | 839.97 | J/mol×K | 995.15 | Joback Method |
| dvisc | 0.0000720 | Pa×s | 795.48 | Joback Method |
| dvisc | 0.0000921 | Pa×s | 742.21 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001223 | Pa×s | 688.95 | Joback Method |
| dvisc | 0.0001703 | Pa×s | 635.68 | Joback Method |
| dvisc | 0.0002520 | Pa×s | 582.41 | Joback Method |
| dvisc | 0.0004036 | Pa×s | 529.15 | Joback Method |
| dvisc | 0.0007181 | Pa×s | 475.88 | 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=U377649&Units=SI |

# 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 |