# Pimelic acid, butyl 4-methoxybenzyl ester

**Inchi:** InChI=1S/C19H28O5/c1-3-4-14-23-18(20)8-6-5-7-9-19(21)24-15-16-10-12-17(22-2)13-11
**InchiKey:** AMQZAWZNKKELEM-UHFFFAOYSA-N
**Formula:** C19H28O5
**SMILES:** CCCCOC(=O)CCCCCC(=O)OCc1ccc(OC)cc1
**Mol. weight [g/mol]:** 336.42

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -360.96 | kJ/mol | Joback Method |
| hf | -832.25 | kJ/mol | Joback Method |
| hfus | 45.38 | kJ/mol | Joback Method |
| hvap | 81.55 | kJ/mol | Joback Method |
| log10ws | -4.80 | | Crippen Method |
| logp | 4.032 | | Crippen Method |
| mcvol | 275.560 | ml/mol | McGowan Method |
| pc | 1422.92 | kPa | Joback Method |
| rinpol | 2613.00 | | NIST Webbook |
| tb | 840.78 | K | Joback Method |
| tc | 1041.20 | K | Joback Method |
| tf | 509.38 | K | Joback Method |
| vc | 1.058 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 848.17 | J/mol×K | 840.78 | Joback Method |
| cpg | 863.62 | J/mol×K | 874.18 | Joback Method |
| cpg | 877.92 | J/mol×K | 907.59 | Joback Method |
| cpg | 891.07 | J/mol×K | 940.99 | Joback Method |
| cpg | 903.09 | J/mol×K | 974.39 | Joback Method |
| cpg | 913.97 | J/mol×K | 1007.79 | Joback Method |
| cpg | 923.73 | J/mol×K | 1041.20 | Joback Method |
| dvisc | 0.0004609 | Pa×s | 509.38 | Joback Method |
| dvisc | 0.0002620 | Pa×s | 564.61 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001648 | Pa×s | 619.85 | Joback Method |
| dvisc | 0.0001118 | Pa×s | 675.08 | Joback Method |
| dvisc | 0.0000804 | Pa×s | 730.31 | Joback Method |
| dvisc | 0.0000606 | Pa×s | 785.55 | Joback Method |
| dvisc | 0.0000474 | Pa×s | 840.78 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U416538&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 |

# 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 |