# Pimelic acid, di(3-(2-methoxyethyl)heptyl) ester

**Inchi:** InChI=1S/C27H52O6/c1-5-7-12-24(16-20-30-3)18-22-32-26(28)14-10-9-11-15-27(29)33-

**InchiKey:** VPZPMJVGCUYRIA-UHFFFAOYSA-N

**Formula:** C27H52O6

**SMILES:** CCCCC(CCOC)CCOC(=O)CCCCCC(=O)OCCC(CCCC)CCOC

**Mol. weight [g/mol]:** 472.70

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -506.26 | kJ/mol | Joback Method |
| hf | -1365.21 | kJ/mol | Joback Method |
| hfus | 66.59 | kJ/mol | Joback Method |
| hvap | 98.05 | kJ/mol | Joback Method |
| log10ws | -6.54 | | Crippen Method |
| logp | 6.489 | | Crippen Method |
| mcvol | 417.910 | ml/mol | McGowan Method |
| pc | 716.45 | kPa | Joback Method |
| rinpol | 3071.00 | | NIST Webbook |
| rinpol | 3071.00 | | NIST Webbook |
| tb | 1013.70 | K | Joback Method |
| tc | 1259.37 | K | Joback Method |
| tf | 552.83 | K | Joback Method |
| vc | 1.619 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1472.76 | J/mol×K | 1013.70 | Joback Method |
| cpg | 1493.07 | J/mol×K | 1054.65 | Joback Method |
| cpg | 1510.89 | J/mol×K | 1095.59 | Joback Method |
| cpg | 1526.25 | J/mol×K | 1136.54 | Joback Method |
| cpg | 1539.18 | J/mol×K | 1177.48 | Joback Method |
| cpg | 1549.70 | J/mol×K | 1218.43 | Joback Method |
| cpg | 1557.86 | J/mol×K | 1259.37 | Joback Method |
| dvisc | 0.0002036 | Pa×s | 552.83 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000859 | Pa×s | 629.64 | Joback Method |
| dvisc | 0.0000437 | Pa×s | 706.45 | Joback Method |
| dvisc | 0.0000254 | Pa×s | 783.26 | Joback Method |
| dvisc | 0.0000163 | Pa×s | 860.08 | Joback Method |
| dvisc | 0.0000112 | Pa×s | 936.89 | Joback Method |
| dvisc | 0.0000082 | Pa×s | 1013.70 | 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=U406791&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 |