# Pimelic acid, isobutyl 2-naphthyl ester

**Inchi:** InChI=1S/C21H26O4/c1-16(2)15-24-20(22)10-4-3-5-11-21(23)25-19-13-12-17-8-6-7-9-18
**InchiKey:** ITQMFUWYVHXOOR-UHFFFAOYSA-N
**Formula:** C21H26O4
**SMILES:** CC(C)COC(=O)CCCCCC(=O)Oc1ccc2ccccc2c1
**Mol. weight [g/mol]:** 342.43

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -134.91 | kJ/mol | Joback Method |
| hf | -555.52 | kJ/mol | Joback Method |
| hfus | 42.87 | kJ/mol | Joback Method |
| hvap | 84.84 | kJ/mol | Joback Method |
| log10ws | -5.98 | | Crippen Method |
| logp | 4.895 | | Crippen Method |
| mcvol | 278.410 | ml/mol | McGowan Method |
| pc | 1510.50 | kPa | Joback Method |
| rinpol | 2735.00 | | NIST Webbook |
| tb | 882.66 | K | Joback Method |
| tc | 1098.28 | K | Joback Method |
| tf | 527.39 | K | Joback Method |
| vc | 1.067 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 861.57 | J/mol×K | 882.66 | Joback Method |
| cpg | 876.41 | J/mol×K | 918.60 | Joback Method |
| cpg | 890.13 | J/mol×K | 954.53 | Joback Method |
| cpg | 902.78 | J/mol×K | 990.47 | Joback Method |
| cpg | 914.42 | J/mol×K | 1026.41 | Joback Method |
| cpg | 925.10 | J/mol×K | 1062.35 | Joback Method |
| cpg | 934.88 | J/mol×K | 1098.28 | Joback Method |
| dvisc | 0.0007083 | Pa×s | 527.39 | Joback Method |
| dvisc | 0.0004187 | Pa×s | 586.60 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002725 | Pa×s | 645.81 | Joback Method |
| dvisc | 0.0001907 | Pa×s | 705.03 | Joback Method |
| dvisc | 0.0001410 | Pa×s | 764.24 | Joback Method |
| dvisc | 0.0001089 | Pa×s | 823.45 | Joback Method |
| dvisc | 0.0000871 | Pa×s | 882.66 | 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=U416708&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 |