# 3-Methoxybenzoic acid, 2-propylpentyl ester

**Inchi:** InChI=1S/C16H24O3/c1-4-7-13(8-5-2)12-19-16(17)14-9-6-10-15(11-14)18-3/h6,9-11,13H
**InchiKey:** IHUDBBOVDBMFEX-UHFFFAOYSA-N
**Formula:** C16H24O3
**SMILES:** CCCC(CCC)COC(=O)c1cccc(OC)c1
**Mol. weight [g/mol]:** 264.36

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -154.74 | kJ/mol | Joback Method |
| hf | -530.81 | kJ/mol | Joback Method |
| hfus | 31.30 | kJ/mol | Joback Method |
| hvap | 65.33 | kJ/mol | Joback Method |
| log10ws | -4.52 | | Crippen Method |
| logp | 4.068 | | Crippen Method |
| mcvol | 225.850 | ml/mol | McGowan Method |
| pc | 1734.67 | kPa | Joback Method |
| rinpol | 1938.00 | | NIST Webbook |
| tb | 695.41 | K | Joback Method |
| tc | 893.53 | K | Joback Method |
| tf | 388.41 | K | Joback Method |
| vc | 0.860 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 628.78 | J/mol×K | 695.41 | Joback Method |
| cpg | 645.72 | J/mol×K | 728.43 | Joback Method |
| cpg | 661.70 | J/mol×K | 761.45 | Joback Method |
| cpg | 676.73 | J/mol×K | 794.47 | Joback Method |
| cpg | 690.82 | J/mol×K | 827.49 | Joback Method |
| cpg | 704.00 | J/mol×K | 860.51 | Joback Method |
| cpg | 716.26 | J/mol×K | 893.53 | Joback Method |
| dvisc | 0.0012264 | Pa×s | 388.41 | Joback Method |
| dvisc | 0.0006106 | Pa×s | 439.58 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0003515 | Pa×s | 490.74 | Joback Method |
| dvisc | 0.0002247 | Pa×s | 541.91 | Joback Method |
| dvisc | 0.0001551 | Pa×s | 593.08 | Joback Method |
| dvisc | 0.0001136 | Pa×s | 644.24 | Joback Method |
| dvisc | 0.0000871 | Pa×s | 695.41 | Joback Method |

# Sources

**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=U374929&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