# Benzoic acid, 3-(neopentyl)oxy-, methyl ester

**Inchi:** InChI=1S/C13H18O3/c1-13(2,3)9-16-11-7-5-6-10(8-11)12(14)15-4/h5-8H,9H2,1-4H3
**InchiKey:** DMMBVVKUHXTPGH-UHFFFAOYSA-N
**Formula:** C13H18O3
**SMILES:** COC(=O)c1cccc(OCC(C)(C)C)c1
**Mol. weight [g/mol]:** 222.28

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -174.72 | kJ/mol | Joback Method |
| hf | -472.36 | kJ/mol | Joback Method |
| hfus | 19.64 | kJ/mol | Joback Method |
| hvap | 57.74 | kJ/mol | Joback Method |
| log10ws | -3.27 | | Crippen Method |
| logp | 2.898 | | Crippen Method |
| mcvol | 183.580 | ml/mol | McGowan Method |
| pc | 2263.26 | kPa | Joback Method |
| rinpol | 1605.00 | | NIST Webbook |
| rinpol | 1605.00 | | NIST Webbook |
| tb | 623.98 | K | Joback Method |
| tc | 837.28 | K | Joback Method |
| tf | 372.02 | K | Joback Method |
| vc | 0.686 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 472.53 | J/mol×K | 623.98 | Joback Method |
| cpg | 542.93 | J/mol×K | 801.73 | Joback Method |
| cpg | 530.70 | J/mol×K | 766.18 | Joback Method |
| cpg | 517.57 | J/mol×K | 730.63 | Joback Method |
| cpg | 503.52 | J/mol×K | 695.08 | Joback Method |
| cpg | 488.51 | J/mol×K | 659.53 | Joback Method |
| cpg | 554.30 | J/mol×K | 837.28 | Joback Method |
| dvisc | 0.0001151 | Pa×s | 623.98 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001492 | Pa×s | 581.99 | Joback Method |
| dvisc | 0.0002015 | Pa×s | 539.99 | Joback Method |
| dvisc | 0.0002862 | Pa×s | 498.00 | Joback Method |
| dvisc | 0.0004337 | Pa×s | 456.01 | Joback Method |
| dvisc | 0.0007150 | Pa×s | 414.01 | Joback Method |
| dvisc | 0.0013196 | Pa×s | 372.02 | 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=U375319&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 |