# Nonanoic acid, 4-benzyloxyphenyl ester

**Other names:** Nonoic acid, 4-benzyloxyphenyl ester
**Inchi:** InChI=1S/C22H28O3/c1-2-3-4-5-6-10-13-22(23)25-21-16-14-20(15-17-21)24-18-19-11-8
**InchiKey:** YFLCPINRCHRNBA-UHFFFAOYSA-N
**Formula:** C22H28O3
**SMILES:** CCCCCCCCC(=O)Oc1ccc(OCc2ccccc2)cc1
**Mol. weight [g/mol]:** 340.46

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 10.63 | kJ/mol | Joback Method |
| hf | -412.84 | kJ/mol | Joback Method |
| hfus | 44.40 | kJ/mol | Joback Method |
| hvap | 81.35 | kJ/mol | Joback Method |
| log10ws | -6.94 | | Crippen Method |
| logp | 5.922 | | Crippen Method |
| mcvol | 286.630 | ml/mol | McGowan Method |
| pc | 1419.71 | kPa | Joback Method |
| rinpol | 2783.00 | | NIST Webbook |
| rinpol | 2783.00 | | NIST Webbook |
| tb | 859.81 | K | Joback Method |
| tc | 1074.51 | K | Joback Method |
| tf | 497.45 | K | Joback Method |
| vc | 1.093 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 883.11 | J/mol×K | 859.81 | Joback Method |
| cpg | 899.53 | J/mol×K | 895.59 | Joback Method |
| cpg | 914.67 | J/mol×K | 931.38 | Joback Method |
| cpg | 928.56 | J/mol×K | 967.16 | Joback Method |
| cpg | 941.26 | J/mol×K | 1002.94 | Joback Method |
| cpg | 952.79 | J/mol×K | 1038.72 | Joback Method |
| cpg | 963.21 | J/mol×K | 1074.51 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0005099 | Pa×s | 497.45 | Joback Method |
| dvisc | 0.0002720 | Pa×s | 557.84 | Joback Method |
| dvisc | 0.0001640 | Pa×s | 618.24 | Joback Method |
| dvisc | 0.0001082 | Pa×s | 678.63 | Joback Method |
| dvisc | 0.0000764 | Pa×s | 739.02 | Joback Method |
| dvisc | 0.0000569 | Pa×s | 799.42 | Joback Method |
| dvisc | 0.0000442 | Pa×s | 859.81 | 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=U358029&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 |