# Nonanoic acid, 4-biphenyl ester

**Inchi:** InChI=1S/C21H26O2/c1-2-3-4-5-6-10-13-21(22)23-20-16-14-19(15-17-20)18-11-8-7-9-12
**InchiKey:** JFIOMVYHCVPMKZ-UHFFFAOYSA-N
**Formula:** C21H26O2
**SMILES:** CCCCCCCCC(=O)Oc1ccc(-c2ccccc2)cc1
**Mol. weight [g/mol]:** 310.43

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 107.21 | kJ/mol | Joback Method |
| hf | -259.98 | kJ/mol | Joback Method |
| hfus | 40.63 | kJ/mol | Joback Method |
| hvap | 76.71 | kJ/mol | Joback Method |
| log10ws | -7.32 | | Crippen Method |
| logp | 6.010 | | Crippen Method |
| mcvol | 266.670 | ml/mol | McGowan Method |
| pc | 1548.78 | kPa | Joback Method |
| rinpol | 2610.00 | | NIST Webbook |
| tb | 814.51 | K | Joback Method |
| tc | 1031.40 | K | Joback Method |
| tf | 463.95 | K | Joback Method |
| vc | 1.020 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 795.54 | J/mol×K | 814.51 | Joback Method |
| cpg | 812.50 | J/mol×K | 850.66 | Joback Method |
| cpg | 828.24 | J/mol×K | 886.81 | Joback Method |
| cpg | 842.80 | J/mol×K | 922.95 | Joback Method |
| cpg | 856.24 | J/mol×K | 959.10 | Joback Method |
| cpg | 868.62 | J/mol×K | 995.25 | Joback Method |
| cpg | 879.99 | J/mol×K | 1031.40 | Joback Method |
| dvisc | 0.0007963 | Pa×s | 463.95 | Joback Method |
| dvisc | 0.0004182 | Pa×s | 522.38 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002500 | Pa×s | 580.80 | Joback Method |
| dvisc | 0.0001642 | Pa×s | 639.23 | Joback Method |
| dvisc | 0.0001157 | Pa×s | 697.66 | Joback Method |
| dvisc | 0.0000861 | Pa×s | 756.08 | Joback Method |
| dvisc | 0.0000668 | Pa×s | 814.51 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U360675&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |