# 4-Oxo-4-phenylbutyric acid, nonyl ester

**Inchi:** InChI=1S/C19H28O3/c1-2-3-4-5-6-7-11-16-22-19(21)15-14-18(20)17-12-9-8-10-13-17/h8
**InchiKey:** OKAOJWPEEOGYIJ-UHFFFAOYSA-N
**Formula:** C19H28O3
**SMILES:** CCCCCCCCCOC(=O)CCC(=O)c1ccccc1
**Mol. weight [g/mol]:** 304.42

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -141.33 | kJ/mol | Joback Method |
| hf | -556.34 | kJ/mol | Joback Method |
| hfus | 43.39 | kJ/mol | Joback Method |
| hvap | 76.07 | kJ/mol | Joback Method |
| log10ws | -5.60 | | Crippen Method |
| logp | 4.943 | | Crippen Method |
| mcvol | 263.820 | ml/mol | McGowan Method |
| pc | 1477.02 | kPa | Joback Method |
| rinpol | 2403.00 | | NIST Webbook |
| tb | 790.96 | K | Joback Method |
| tc | 989.24 | K | Joback Method |
| tf | 452.40 | K | Joback Method |
| vc | 1.022 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 790.41 | J/mol×K | 790.96 | Joback Method |
| cpg | 806.84 | J/mol×K | 824.01 | Joback Method |
| cpg | 822.21 | J/mol×K | 857.05 | Joback Method |
| cpg | 836.58 | J/mol×K | 890.10 | Joback Method |
| cpg | 849.98 | J/mol×K | 923.14 | Joback Method |
| cpg | 862.43 | J/mol×K | 956.19 | Joback Method |
| cpg | 873.99 | J/mol×K | 989.24 | Joback Method |
| dvisc | 0.0011097 | Pa×s | 452.40 | Joback Method |
| dvisc | 0.0005659 | Pa×s | 508.83 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0003301 | Pa×s | 565.25 | Joback Method |
| dvisc | 0.0002123 | Pa×s | 621.68 | Joback Method |
| dvisc | 0.0001470 | Pa×s | 678.11 | Joback Method |
| dvisc | 0.0001077 | Pa×s | 734.53 | Joback Method |
| dvisc | 0.0000825 | Pa×s | 790.96 | Joback Method |

# Sources

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|---|---|
| **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=U405980&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |