# Sebacic acid, pentyl 2-phenylphenyl ester

**Inchi:** InChI=1S/C27H36O4/c1-2-3-15-22-30-26(28)20-11-6-4-5-7-12-21-27(29)31-25-19-14-13
**InchiKey:** AHLVYHNNJAEULO-UHFFFAOYSA-N
**Formula:** C27H36O4
**SMILES:** CCCCCOC(=O)CCCCCCCCC(=O)Oc1ccccc1-c1ccccc1
**Mol. weight [g/mol]:** 424.57

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -76.19 | kJ/mol | Joback Method |
| hf | -628.62 | kJ/mol | Joback Method |
| hfus | 58.95 | kJ/mol | Joback Method |
| hvap | 99.22 | kJ/mol | Joback Method |
| log10ws | -8.69 | | Crippen Method |
| logp | 7.113 | | Crippen Method |
| mcvol | 358.650 | ml/mol | McGowan Method |
| pc | 1060.33 | kPa | Joback Method |
| rinpol | 3174.00 | | NIST Webbook |
| rinpol | 3174.00 | | NIST Webbook |
| tb | 1028.08 | K | Joback Method |
| tc | 1259.02 | K | Joback Method |
| tf | 603.73 | K | Joback Method |
| vc | 1.379 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1198.95 | J/mol×K | 1028.08 | Joback Method |
| cpg | 1213.64 | J/mol×K | 1066.57 | Joback Method |
| cpg | 1226.81 | J/mol×K | 1105.06 | Joback Method |
| cpg | 1238.53 | J/mol×K | 1143.55 | Joback Method |
| cpg | 1248.86 | J/mol×K | 1182.04 | Joback Method |
| cpg | 1257.89 | J/mol×K | 1220.53 | Joback Method |
| cpg | 1265.69 | J/mol×K | 1259.02 | Joback Method |
| dvisc | 0.0002386 | Pa×s | 603.73 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001276 | Pa×s | 674.46 | Joback Method |
| dvisc | 0.0000768 | Pa×s | 745.18 | Joback Method |
| dvisc | 0.0000505 | Pa×s | 815.90 | Joback Method |
| dvisc | 0.0000355 | Pa×s | 886.63 | Joback Method |
| dvisc | 0.0000263 | Pa×s | 957.35 | Joback Method |
| dvisc | 0.0000203 | Pa×s | 1028.08 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U355065&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 |