# Sebacic acid, heptyl 2-phenylphenyl ester

**Inchi:** InChI=1S/C29H40O4/c1-2-3-4-9-17-24-32-28(30)22-13-7-5-6-8-14-23-29(31)33-27-21-16
**InchiKey:** ZLKDRFKOVJJTGE-UHFFFAOYSA-N
**Formula:** C29H40O4
**SMILES:** CCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccccc1-c1ccccc1
**Mol. weight [g/mol]:** 452.63

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -59.35 | kJ/mol | Joback Method |
| hf | -669.90 | kJ/mol | Joback Method |
| hfus | 64.13 | kJ/mol | Joback Method |
| hvap | 103.67 | kJ/mol | Joback Method |
| log10ws | -9.53 | | Crippen Method |
| logp | 7.893 | | Crippen Method |
| mcvol | 386.830 | ml/mol | McGowan Method |
| pc | 939.22 | kPa | Joback Method |
| rinpol | 3379.00 | | NIST Webbook |
| tb | 1073.84 | K | Joback Method |
| tc | 1315.50 | K | Joback Method |
| tf | 626.27 | K | Joback Method |
| vc | 1.492 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1322.46 | J/mol×K | 1073.84 | Joback Method |
| cpg | 1337.42 | J/mol×K | 1114.12 | Joback Method |
| cpg | 1350.72 | J/mol×K | 1154.39 | Joback Method |
| cpg | 1362.43 | J/mol×K | 1194.67 | Joback Method |
| cpg | 1372.67 | J/mol×K | 1234.94 | Joback Method |
| cpg | 1381.51 | J/mol×K | 1275.22 | Joback Method |
| cpg | 1389.06 | J/mol×K | 1315.50 | Joback Method |
| dvisc | 0.0001861 | Pa×s | 626.27 | Joback Method |
| dvisc | 0.0000977 | Pa×s | 700.87 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000580 | Pa×s | 775.46 | Joback Method |
| dvisc | 0.0000378 | Pa×s | 850.05 | Joback Method |
| dvisc | 0.0000264 | Pa×s | 924.65 | Joback Method |
| dvisc | 0.0000194 | Pa×s | 999.24 | Joback Method |
| dvisc | 0.0000149 | Pa×s | 1073.84 | Joback Method |

# Sources

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|---|---|
| **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=U355068&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |