# Sebacic acid, heptyl 2-phenoxyethyl ester

**Inchi:** InChI=1S/C25H40O5/c1-2-3-4-9-15-20-29-24(26)18-13-7-5-6-8-14-19-25(27)30-22-21-28
**InchiKey:** YHJAQEDFWIYTIE-UHFFFAOYSA-N
**Formula:** C25H40O5
**SMILES:** CCCCCCCOC(=O)CCCCCCCCC(=O)OCCOc1ccccc1
**Mol. weight [g/mol]:** 420.58

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -300.81 | kJ/mol | Joback Method |
| hf | -944.62 | kJ/mol | Joback Method |
| hfus | 61.31 | kJ/mol | Joback Method |
| hvap | 94.24 | kJ/mol | Joback Method |
| log10ws | -6.85 | | Crippen Method |
| logp | 6.243 | | Crippen Method |
| mcvol | 360.100 | ml/mol | McGowan Method |
| pc | 969.28 | kPa | Joback Method |
| rinpol | 3050.00 | | NIST Webbook |
| rinpol | 3050.00 | | NIST Webbook |
| tb | 973.08 | K | Joback Method |
| tc | 1191.68 | K | Joback Method |
| tf | 564.48 | K | Joback Method |
| vc | 1.393 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1211.60 | J/mol×K | 973.08 | Joback Method |
| cpg | 1279.52 | J/mol×K | 1155.25 | Joback Method |
| cpg | 1269.00 | J/mol×K | 1118.82 | Joback Method |
| cpg | 1256.98 | J/mol×K | 1082.38 | Joback Method |
| cpg | 1243.44 | J/mol×K | 1045.95 | Joback Method |
| cpg | 1228.33 | J/mol×K | 1009.51 | Joback Method |
| cpg | 1288.58 | J/mol×K | 1191.68 | Joback Method |
| dvisc | 0.0000191 | Pa×s | 973.08 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000252 | Pa×s | 904.98 | Joback Method |
| dvisc | 0.0000347 | Pa×s | 836.88 | Joback Method |
| dvisc | 0.0000505 | Pa×s | 768.78 | Joback Method |
| dvisc | 0.0000792 | Pa×s | 700.68 | Joback Method |
| dvisc | 0.0001368 | Pa×s | 632.58 | Joback Method |
| dvisc | 0.0002695 | Pa×s | 564.48 | 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=U380785&Units=SI |

# 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 |