# Sebacic acid, (2-(cyclohexenyl-3)-1-phenyl)ethyl isohexyl ester

**Inchi:** InChI=1S/C30H46O4/c1-25(2)16-15-23-33-29(31)21-13-5-3-4-6-14-22-30(32)34-28(27-1

**InchiKey:** ALKPWRDTORZZCP-UHFFFAOYSA-N

**Formula:** C30H46O4

**SMILES:** CC(C)CCCOC(=O)CCCCCCCCC(=O)OC(CC1C=CCCC1)c1ccccc1

**Mol. weight [g/mol]:** 470.68

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -104.18 | kJ/mol | Joback Method |
| hf | -814.06 | kJ/mol | Joback Method |
| hfus | 59.08 | kJ/mol | Joback Method |
| hvap | 102.91 | kJ/mol | Joback Method |
| log10ws | -8.93 | | Crippen Method |
| logp | 8.117 | | Crippen Method |
| mcvol | 409.520 | ml/mol | McGowan Method |
| pc | 855.96 | kPa | Joback Method |
| rinpol | 3450.00 | | NIST Webbook |
| tb | 1082.89 | K | Joback Method |
| tc | 1327.11 | K | Joback Method |
| tf | 576.74 | K | Joback Method |
| vc | 1.562 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1457.82 | J/mol×K | 1082.89 | Joback Method |
| cpg | 1520.11 | J/mol×K | 1286.41 | Joback Method |
| cpg | 1511.15 | J/mol×K | 1245.70 | Joback Method |
| cpg | 1500.55 | J/mol×K | 1205.00 | Joback Method |
| cpg | 1488.19 | J/mol×K | 1164.30 | Joback Method |
| cpg | 1473.98 | J/mol×K | 1123.59 | Joback Method |
| cpg | 1527.54 | J/mol×K | 1327.11 | Joback Method |
| dvisc | 0.0000110 | Pa×s | 1082.89 | Joback Method |
| dvisc | 0.0000151 | Pa×s | 998.53 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000219 | Pa×s | 914.17 | Joback Method |
| dvisc | 0.0000341 | Pa×s | 829.81 | Joback Method |
| dvisc | 0.0000590 | Pa×s | 745.46 | Joback Method |
| dvisc | 0.0001171 | Pa×s | 661.10 | Joback Method |
| dvisc | 0.0002844 | Pa×s | 576.74 | 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=U354421&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 |