# Sebacic acid, isohexyl 4-phenylphenyl ester

**Inchi:** InChI=1S/C28H38O4/c1-23(2)13-12-22-31-27(29)16-10-5-3-4-6-11-17-28(30)32-26-20-1
**InchiKey:** VRVRFIJXMDXAAT-UHFFFAOYSA-N
**Formula:** C28H38O4
**SMILES:** CC(C)CCCOC(=O)CCCCCCCCC(=O)Oc1ccc(-c2ccccc2)cc1
**Mol. weight [g/mol]:** 438.60

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -70.21 | kJ/mol | Joback Method |
| hf | -654.54 | kJ/mol | Joback Method |
| hfus | 58.02 | kJ/mol | Joback Method |
| hvap | 101.06 | kJ/mol | Joback Method |
| log10ws | -8.87 | | Crippen Method |
| logp | 7.359 | | Crippen Method |
| mcvol | 372.740 | ml/mol | McGowan Method |
| pc | 1002.08 | kPa | Joback Method |
| rinpol | 3544.00 | | NIST Webbook |
| tb | 1050.52 | K | Joback Method |
| tc | 1286.15 | K | Joback Method |
| tf | 600.00 | K | Joback Method |
| vc | 1.429 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1260.78 | J/mol×K | 1050.52 | Joback Method |
| cpg | 1275.50 | J/mol×K | 1089.79 | Joback Method |
| cpg | 1288.62 | J/mol×K | 1129.06 | Joback Method |
| cpg | 1300.21 | J/mol×K | 1168.34 | Joback Method |
| cpg | 1310.36 | J/mol×K | 1207.61 | Joback Method |
| cpg | 1319.15 | J/mol×K | 1246.88 | Joback Method |
| cpg | 1326.66 | J/mol×K | 1286.15 | Joback Method |
| dvisc | 0.0002284 | Pa×s | 600.00 | Joback Method |
| dvisc | 0.0001143 | Pa×s | 675.09 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000657 | Pa×s | 750.17 | Joback Method |
| dvisc | 0.0000417 | Pa×s | 825.26 | Joback Method |
| dvisc | 0.0000286 | Pa×s | 900.35 | Joback Method |
| dvisc | 0.0000208 | Pa×s | 975.43 | Joback Method |
| dvisc | 0.0000158 | Pa×s | 1050.52 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U355254&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

**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