# Sebacic acid, isobutyl 4-phenoxybenzyl ester

**Inchi:** InChI=1S/C27H36O5/c1-22(2)20-30-26(28)14-10-5-3-4-6-11-15-27(29)31-21-23-16-18-2
**InchiKey:** XUNJNWYFEMJHNK-UHFFFAOYSA-N
**Formula:** C27H36O5
**SMILES:** CC(C)COC(=O)CCCCCCCCC(=O)OCc1ccc(Oc2ccccc2)cc1
**Mol. weight [g/mol]:** 440.57

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -183.63 | kJ/mol | Joback Method |
| hf | -766.12 | kJ/mol | Joback Method |
| hfus | 56.62 | kJ/mol | Joback Method |
| hvap | 101.24 | kJ/mol | Joback Method |
| log10ws | -7.33 | | Crippen Method |
| logp | 6.842 | | Crippen Method |
| mcvol | 364.520 | ml/mol | McGowan Method |
| pc | 1054.14 | kPa | Joback Method |
| rinpol | 3297.00 | | NIST Webbook |
| tb | 1050.06 | K | Joback Method |
| tc | 1285.62 | K | Joback Method |
| tf | 610.96 | K | Joback Method |
| vc | 1.391 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1226.04 | J/mol×K | 1050.06 | Joback Method |
| cpg | 1276.07 | J/mol×K | 1246.36 | Joback Method |
| cpg | 1269.37 | J/mol×K | 1207.10 | Joback Method |
| cpg | 1261.07 | J/mol×K | 1167.84 | Joback Method |
| cpg | 1251.12 | J/mol×K | 1128.58 | Joback Method |
| cpg | 1239.46 | J/mol×K | 1089.32 | Joback Method |
| cpg | 1281.23 | J/mol×K | 1285.62 | Joback Method |
| dvisc | 0.0000135 | Pa×s | 1050.06 | Joback Method |
| dvisc | 0.0000177 | Pa×s | 976.88 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000242 | Pa×s | 903.69 | Joback Method |
| dvisc | 0.0000349 | Pa×s | 830.51 | Joback Method |
| dvisc | 0.0000542 | Pa×s | 757.33 | Joback Method |
| dvisc | 0.0000922 | Pa×s | 684.14 | Joback Method |
| dvisc | 0.0001782 | Pa×s | 610.96 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U355038&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