# Sebacic acid, dodecyl 3-methylbutyl ester

**Inchi:** InChI=1S/C27H52O4/c1-4-5-6-7-8-9-10-13-16-19-23-30-26(28)20-17-14-11-12-15-18-21
**InchiKey:** BWJJFNJWTQRNRG-UHFFFAOYSA-N
**Formula:** C27H52O4
**SMILES:** CCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCC(C)C
**Mol. weight [g/mol]:** 440.70

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -293.82 | kJ/mol | Joback Method |
| hf | -1095.49 | kJ/mol | Joback Method |
| hfus | 67.74 | kJ/mol | Joback Method |
| hvap | 93.62 | kJ/mol | Joback Method |
| log10ws | -8.61 | | Crippen Method |
| logp | 8.161 | | Crippen Method |
| mcvol | 406.170 | ml/mol | McGowan Method |
| pc | 726.53 | kPa | Joback Method |
| rinpol | 3044.00 | | NIST Webbook |
| rinpol | 3044.00 | | NIST Webbook |
| tb | 969.30 | K | Joback Method |
| tc | 1196.72 | K | Joback Method |
| tf | 523.37 | K | Joback Method |
| vc | 1.589 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1410.04 | J/mol×K | 969.30 | Joback Method |
| cpg | 1431.86 | J/mol×K | 1007.20 | Joback Method |
| cpg | 1451.85 | J/mol×K | 1045.11 | Joback Method |
| cpg | 1470.06 | J/mol×K | 1083.01 | Joback Method |
| cpg | 1486.55 | J/mol×K | 1120.91 | Joback Method |
| cpg | 1501.39 | J/mol×K | 1158.81 | Joback Method |
| cpg | 1514.63 | J/mol×K | 1196.72 | Joback Method |
| dvisc | 0.0004080 | Pa×s | 523.37 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001723 | Pa×s | 597.69 | Joback Method |
| dvisc | 0.0000881 | Pa×s | 672.01 | Joback Method |
| dvisc | 0.0000515 | Pa×s | 746.34 | Joback Method |
| dvisc | 0.0000331 | Pa×s | 820.66 | Joback Method |
| dvisc | 0.0000230 | Pa×s | 894.98 | Joback Method |
| dvisc | 0.0000168 | Pa×s | 969.30 | 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=U355376&Units=SI |

# 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 |