# Sebacic acid, butyl cis-non-3-enyl ester

**Inchi:** InChI=1S/C23H42O4/c1-3-5-7-8-11-14-17-21-27-23(25)19-16-13-10-9-12-15-18-22(24)2
**InchiKey:** POOZEKMXNFQSNT-KAMYIIQDSA-N
**Formula:** C23H42O4
**SMILES:** CCCCCC=CCCOC(=O)CCCCCCCCC(=O)OCCCC
**Mol. weight [g/mol]:** 382.58

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -244.84 | kJ/mol | Joback Method |
| hf | -890.43 | kJ/mol | Joback Method |
| hfus | 61.10 | kJ/mol | Joback Method |
| hvap | 85.06 | kJ/mol | Joback Method |
| log10ws | -7.03 | | Crippen Method |
| logp | 6.520 | | Crippen Method |
| mcvol | 345.510 | ml/mol | McGowan Method |
| pc | 928.37 | kPa | Joback Method |
| rinpol | 2665.00 | | NIST Webbook |
| tb | 882.38 | K | Joback Method |
| tc | 1080.29 | K | Joback Method |
| tf | 488.21 | K | Joback Method |
| vc | 1.351 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1127.87 | J/mol×K | 882.38 | Joback Method |
| cpg | 1146.91 | J/mol×K | 915.36 | Joback Method |
| cpg | 1164.75 | J/mol×K | 948.35 | Joback Method |
| cpg | 1181.44 | J/mol×K | 981.33 | Joback Method |
| cpg | 1197.00 | J/mol×K | 1014.32 | Joback Method |
| cpg | 1211.47 | J/mol×K | 1047.30 | Joback Method |
| cpg | 1224.91 | J/mol×K | 1080.29 | Joback Method |
| dvisc | 0.0005530 | Pa×s | 488.21 | Joback Method |
| dvisc | 0.0002548 | Pa×s | 553.90 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001384 | Pa×s | 619.60 | Joback Method |
| dvisc | 0.0000845 | Pa×s | 685.30 | Joback Method |
| dvisc | 0.0000562 | Pa×s | 750.99 | Joback Method |
| dvisc | 0.0000400 | Pa×s | 816.68 | Joback Method |
| dvisc | 0.0000299 | Pa×s | 882.38 | 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=U355921&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 |