# Sebacic acid, di(3-methylbut-2-enyl) ester

**Inchi:** InChI=1S/C20H34O4/c1-17(2)13-15-23-19(21)11-9-7-5-6-8-10-12-20(22)24-16-14-18(3)4
**InchiKey:** SBTCSFVKCOKYIX-UHFFFAOYSA-N
**Formula:** C20H34O4
**SMILES:** CC(C)=CCOC(=O)CCCCCCCCC(=O)OCC=C(C)C
**Mol. weight [g/mol]:** 338.48

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -206.98 | kJ/mol | Joback Method |
| hf | -730.87 | kJ/mol | Joback Method |
| hfus | 50.91 | kJ/mol | Joback Method |
| hvap | 78.50 | kJ/mol | Joback Method |
| log10ws | -5.63 | | Crippen Method |
| logp | 5.126 | | Crippen Method |
| mcvol | 298.940 | ml/mol | McGowan Method |
| pc | 1163.25 | kPa | Joback Method |
| rinpol | 2427.00 | | NIST Webbook |
| tb | 817.66 | K | Joback Method |
| tc | 1008.62 | K | Joback Method |
| tf | 421.40 | K | Joback Method |
| vc | 1.165 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 917.59 | J/mol×K | 817.66 | Joback Method |
| cpg | 934.92 | J/mol×K | 849.49 | Joback Method |
| cpg | 951.28 | J/mol×K | 881.31 | Joback Method |
| cpg | 966.72 | J/mol×K | 913.14 | Joback Method |
| cpg | 981.28 | J/mol×K | 944.96 | Joback Method |
| cpg | 994.99 | J/mol×K | 976.79 | Joback Method |
| cpg | 1007.90 | J/mol×K | 1008.62 | 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=U355886&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |