# Succinic acid, 2-iodobenzyl hexadecyl ester

**Inchi:** InChI=1S/C27H43IO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-22-31-26(29)20-21-27(30)3
**InchiKey:** YAIJJUYDHUZESW-UHFFFAOYSA-N
**Formula:** C27H43IO4
**SMILES:** CCCCCCCCCCCCCCCCCOC(=O)CCC(=O)OCc1ccccc1I
**Mol. weight [g/mol]:** 558.53

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -130.48 | kJ/mol | Joback Method |
| hf | -788.28 | kJ/mol | Joback Method |
| hfus | 69.32 | kJ/mol | Joback Method |
| hvap | 106.32 | kJ/mol | Joback Method |
| log10ws | -9.60 | | Crippen Method |
| logp | 8.139 | | Crippen Method |
| mcvol | 408.230 | ml/mol | McGowan Method |
| pc | 852.97 | kPa | Joback Method |
| rinpol | 3542.00 | | NIST Webbook |
| rinpol | 3542.00 | | NIST Webbook |
| tb | 1094.54 | K | Joback Method |
| tc | 1344.07 | K | Joback Method |
| tf | 635.37 | K | Joback Method |
| vc | 1.575 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1356.74 | J/mol×K | 1094.54 | Joback Method |
| cpg | 1372.24 | J/mol×K | 1136.13 | Joback Method |
| cpg | 1386.11 | J/mol×K | 1177.72 | Joback Method |
| cpg | 1398.45 | J/mol×K | 1219.31 | Joback Method |
| cpg | 1409.35 | J/mol×K | 1260.89 | Joback Method |
| cpg | 1418.90 | J/mol×K | 1302.48 | Joback Method |
| cpg | 1427.21 | J/mol×K | 1344.07 | Joback Method |
| dvisc | 0.0001704 | Pa×s | 635.37 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000877 | Pa×s | 711.90 | Joback Method |
| dvisc | 0.0000513 | Pa×s | 788.43 | Joback Method |
| dvisc | 0.0000330 | Pa×s | 864.95 | Joback Method |
| dvisc | 0.0000228 | Pa×s | 941.48 | Joback Method |
| dvisc | 0.0000167 | Pa×s | 1018.01 | Joback Method |
| dvisc | 0.0000128 | Pa×s | 1094.54 | Joback Method |

# Sources

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|---|---|
| **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=U381113&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |