# Succinic acid, di(2-nitrobenzyl) ester

**Inchi:** InChI=1S/C18H16N2O8/c21-17(27-11-13-5-1-3-7-15(13)19(23)24)9-10-18(22)28-12-14-6
**InchiKey:** UACDKYUTVLNPJH-UHFFFAOYSA-N
**Formula:** C18H16N2O8
**SMILES:** O=C(CCC(=O)OCc1ccccc1[N+](=O)[O-])OCc1ccccc1[N+](=O)[O-]
**Mol. weight [g/mol]:** 388.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -90.50 | kJ/mol | Joback Method |
| hf | -475.85 | kJ/mol | Joback Method |
| hfus | 57.98 | kJ/mol | Joback Method |
| hvap | 113.03 | kJ/mol | Joback Method |
| log10ws | -5.58 | | Crippen Method |
| logp | 3.070 | | Crippen Method |
| mcvol | 266.680 | ml/mol | McGowan Method |
| pc | 2069.88 | kPa | Joback Method |
| rinpol | 3131.00 | | NIST Webbook |
| rinpol | 3131.00 | | NIST Webbook |
| tb | 1130.82 | K | Joback Method |
| tc | 1397.42 | K | Joback Method |
| tf | 802.04 | K | Joback Method |
| vc | 1.040 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 836.51 | J/mol×K | 1130.82 | Joback Method |
| cpg | 841.63 | J/mol×K | 1175.25 | Joback Method |
| cpg | 845.28 | J/mol×K | 1219.69 | Joback Method |
| cpg | 847.53 | J/mol×K | 1264.12 | Joback Method |
| cpg | 848.42 | J/mol×K | 1308.55 | Joback Method |
| cpg | 848.04 | J/mol×K | 1352.99 | Joback Method |
| cpg | 846.43 | J/mol×K | 1397.42 | 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=U380904&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **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 |

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