# Succinic acid, heptyl 3-nitrobenzyl ester

**Inchi:** InChI=1S/C18H25NO6/c1-2-3-4-5-6-12-24-17(20)10-11-18(21)25-14-15-8-7-9-16(13-15)
**InchiKey:** GDKHHLYNKSSESL-UHFFFAOYSA-N
**Formula:** C18H25NO6
**SMILES:** CCCCCCCOC(=O)CCC(=O)OCc1cccc([N+](=O)[O-])c1
**Mol. weight [g/mol]:** 351.39

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -228.83 | kJ/mol | Joback Method |
| hf | -690.15 | kJ/mol | Joback Method |
| hfus | 52.96 | kJ/mol | Joback Method |
| hvap | 93.50 | kJ/mol | Joback Method |
| log10ws | -5.33 | | Crippen Method |
| logp | 3.932 | | Crippen Method |
| mcvol | 273.020 | ml/mol | McGowan Method |
| pc | 1567.23 | kPa | Joback Method |
| rinpol | 2680.00 | | NIST Webbook |
| rinpol | 2680.00 | | NIST Webbook |
| tb | 947.32 | K | Joback Method |
| tc | 1169.79 | K | Joback Method |
| tf | 619.49 | K | Joback Method |
| vc | 1.065 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 870.47 | J/mol×K | 947.32 | Joback Method |
| cpg | 882.84 | J/mol×K | 984.40 | Joback Method |
| cpg | 893.96 | J/mol×K | 1021.48 | Joback Method |
| cpg | 903.85 | J/mol×K | 1058.56 | Joback Method |
| cpg | 912.55 | J/mol×K | 1095.64 | Joback Method |
| cpg | 920.08 | J/mol×K | 1132.72 | Joback Method |
| cpg | 926.47 | J/mol×K | 1169.79 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U381692&Units=SI |
| **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 |

# 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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