# Succinic acid, 3,5-dinitro-2-methylbenzyl propyl ester

**Inchi:** InChI=1S/C15H18N2O8/c1-3-6-24-14(18)4-5-15(19)25-9-11-7-12(16(20)21)8-13(10(11)2

**InchiKey:** RYBIKFNJUANPDA-UHFFFAOYSA-N

**Formula:** C15H18N2O8

**SMILES:** CCCOC(=O)CCC(=O)OCc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1C

**Mol. weight [g/mol]:** 354.31

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -237.80 | kJ/mol | Joback Method |
| hf | -661.93 | kJ/mol | Joback Method |
| hfus | 55.78 | kJ/mol | Joback Method |
| hvap | 104.74 | kJ/mol | Joback Method |
| log10ws | -4.78 | | Crippen Method |
| logp | 2.588 | | Crippen Method |
| mcvol | 248.170 | ml/mol | McGowan Method |
| pc | 1964.82 | kPa | Joback Method |
| rinpol | 2645.00 | | NIST Webbook |
| rinpol | 2645.00 | | NIST Webbook |
| tb | 1040.48 | K | Joback Method |
| tc | 1286.37 | K | Joback Method |
| tf | 754.33 | K | Joback Method |
| vc | 0.980 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 782.00 | J/mol×K | 1040.48 | Joback Method |
| cpg | 789.64 | J/mol×K | 1081.46 | Joback Method |
| cpg | 795.86 | J/mol×K | 1122.44 | Joback Method |
| cpg | 800.67 | J/mol×K | 1163.43 | Joback Method |
| cpg | 804.09 | J/mol×K | 1204.41 | Joback Method |
| cpg | 806.13 | J/mol×K | 1245.39 | Joback Method |
| cpg | 806.81 | J/mol×K | 1286.37 | 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=U381005&Units=SI |

# 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 |