# Succinic acid, 2-(dimethylamino)ethyl 3,5-dimethylphenyl ester

**Inchi:** InChI=1S/C16H23NO4/c1-12-9-13(2)11-14(10-12)21-16(19)6-5-15(18)20-8-7-17(3)4/h9-1

**InchiKey:** LTKZDRFEXRDINB-UHFFFAOYSA-N

**Formula:** C16H23NO4

**SMILES:** Cc1cc(C)cc(OC(=O)CCC(=O)OCCN(C)C)c1

**Mol. weight [g/mol]:** 293.36

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -180.07 | kJ/mol | Joback Method |
| hf | -582.05 | kJ/mol | Joback Method |
| hfus | 39.05 | kJ/mol | Joback Method |
| hvap | 75.16 | kJ/mol | Joback Method |
| log10ws | -2.68 | | Crippen Method |
| logp | 2.094 | | Crippen Method |
| mcvol | 237.400 | ml/mol | McGowan Method |
| pc | 1790.91 | kPa | Joback Method |
| rinpol | 2182.00 | | NIST Webbook |
| tb | 767.14 | K | Joback Method |
| tc | 968.23 | K | Joback Method |
| tf | 498.33 | K | Joback Method |
| vc | 0.889 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 688.28 | J/mol×K | 767.14 | Joback Method |
| cpg | 703.39 | J/mol×K | 800.65 | Joback Method |
| cpg | 717.51 | J/mol×K | 834.17 | Joback Method |
| cpg | 730.64 | J/mol×K | 867.68 | Joback Method |
| cpg | 742.82 | J/mol×K | 901.20 | Joback Method |
| cpg | 754.04 | J/mol×K | 934.71 | Joback Method |
| cpg | 764.34 | J/mol×K | 968.23 | Joback Method |

# Sources

| | |
|---|---|
| **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=U360729&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |