# Isophthalic acid, 3,4-dimethylphenyl undecyl ester

**Inchi:** InChI=1S/C27H36O4/c1-4-5-6-7-8-9-10-11-12-18-30-26(28)23-14-13-15-24(20-23)27(29
**InchiKey:** RXJPIBLNYBSQBM-UHFFFAOYSA-N
**Formula:** C27H36O4
**SMILES:** CCCCCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccc(C)c(C)c2)c1
**Mol. weight [g/mol]:** 424.57

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -95.45 | kJ/mol | Joback Method |
| hf | -651.56 | kJ/mol | Joback Method |
| hfus | 58.17 | kJ/mol | Joback Method |
| hvap | 100.55 | kJ/mol | Joback Method |
| log10ws | -8.94 | | Crippen Method |
| logp | 7.210 | | Crippen Method |
| mcvol | 358.650 | ml/mol | McGowan Method |
| pc | 1039.91 | kPa | Joback Method |
| rinpol | 3421.00 | | NIST Webbook |
| rinpol | 3421.00 | | NIST Webbook |
| tb | 1038.04 | K | Joback Method |
| tc | 1271.10 | K | Joback Method |
| tf | 628.77 | K | Joback Method |
| vc | 1.379 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1196.79 | J/mol×K | 1038.04 | Joback Method |
| cpg | 1252.82 | J/mol×K | 1232.26 | Joback Method |
| cpg | 1244.61 | J/mol×K | 1193.42 | Joback Method |
| cpg | 1234.96 | J/mol×K | 1154.57 | Joback Method |
| cpg | 1223.81 | J/mol×K | 1115.73 | Joback Method |
| cpg | 1211.11 | J/mol×K | 1076.88 | Joback Method |
| cpg | 1259.63 | J/mol×K | 1271.10 | Joback Method |
| dvisc | 0.0000214 | Pa×s | 1038.04 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000272 | Pa×s | 969.83 | Joback Method |
| dvisc | 0.0000357 | Pa×s | 901.62 | Joback Method |
| dvisc | 0.0000491 | Pa×s | 833.40 | Joback Method |
| dvisc | 0.0000714 | Pa×s | 765.19 | Joback Method |
| dvisc | 0.0001118 | Pa×s | 696.98 | Joback Method |
| dvisc | 0.0001928 | Pa×s | 628.77 | Joback Method |

# Sources

| | |
|---|---|
| **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=U344448&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

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