# Isophthalic acid, 2-methylphenyl nonyl ester

**Inchi:** InChI=1S/C24H30O4/c1-3-4-5-6-7-8-11-17-27-23(25)20-14-12-15-21(18-20)24(26)28-22
**InchiKey:** YBEDUQRVBJAEOF-UHFFFAOYSA-N
**Formula:** C24H30O4
**SMILES:** CCCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2C)c1
**Mol. weight [g/mol]:** 382.49

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -111.08 | kJ/mol | Joback Method |
| hf | -578.17 | kJ/mol | Joback Method |
| hfus | 50.79 | kJ/mol | Joback Method |
| hvap | 93.21 | kJ/mol | Joback Method |
| log10ws | -7.63 | | Crippen Method |
| logp | 6.122 | | Crippen Method |
| mcvol | 316.380 | ml/mol | McGowan Method |
| pc | 1277.33 | kPa | Joback Method |
| rinpol | 3062.00 | | NIST Webbook |
| rinpol | 3062.00 | | NIST Webbook |
| tb | 964.42 | K | Joback Method |
| tc | 1187.99 | K | Joback Method |
| tf | 582.44 | K | Joback Method |
| vc | 1.212 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1015.71 | J/mol×K | 964.42 | Joback Method |
| cpg | 1030.03 | J/mol×K | 1001.68 | Joback Method |
| cpg | 1042.95 | J/mol×K | 1038.94 | Joback Method |
| cpg | 1054.50 | J/mol×K | 1076.21 | Joback Method |
| cpg | 1064.74 | J/mol×K | 1113.47 | Joback Method |
| cpg | 1073.72 | J/mol×K | 1150.73 | Joback Method |
| cpg | 1081.47 | J/mol×K | 1187.99 | Joback Method |
| dvisc | 0.0003008 | Pa×s | 582.44 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0001730 | Pa×s | 646.10 | Joback Method |
| dvisc | 0.0001098 | Pa×s | 709.77 | Joback Method |
| dvisc | 0.0000752 | Pa×s | 773.43 | Joback Method |
| dvisc | 0.0000545 | Pa×s | 837.09 | Joback Method |
| dvisc | 0.0000413 | Pa×s | 900.76 | Joback Method |
| dvisc | 0.0000325 | Pa×s | 964.42 | Joback Method |

# Sources

| | |
|---|---|
| **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=U344352&Units=SI |

# 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 |

Latest version available from:
https://www.chemeo.com/cid/86-784-7/Isophthalic-acid-2-methylphenyl-nonyl-ester.pdf
Generated by Cheméo on 2024-10-12 04:41:26.622137215 +0000 UTC m=+3288949.259106514.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.