# Isophthalic acid, 2,7-dimethyloct-7-en-5-yn-4-yl propyl ester

**Inchi:** InChI=1S/C21H26O4/c1-6-12-24-20(22)17-8-7-9-18(14-17)21(23)25-19(13-16(4)5)11-10

**InchiKey:** DSSCKIMHICUIQX-UHFFFAOYSA-N

**Formula:** C21H26O4

**SMILES:** C=C(C)C#CC(CC(C)C)OC(=O)c1cccc(C(=O)OCCC)c1

**Mol. weight [g/mol]:** 342.43

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 38.09 | kJ/mol | Joback Method |
| hf | -363.93 | kJ/mol | Joback Method |
| hfus | 42.86 | kJ/mol | Joback Method |
| hvap | 84.38 | kJ/mol | Joback Method |
| log10ws | -6.08 | | Crippen Method |
| logp | 4.404 | | Crippen Method |
| mcvol | 284.970 | ml/mol | McGowan Method |
| pc | 1475.88 | kPa | Joback Method |
| rinpol | 2410.00 | | NIST Webbook |
| rinpol | 2410.00 | | NIST Webbook |
| tb | 868.80 | K | Joback Method |
| tc | 1089.27 | K | Joback Method |
| tf | 570.07 | K | Joback Method |
| vc | 1.083 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 857.54 | J/mol×K | 868.80 | Joback Method |
| cpg | 873.10 | J/mol×K | 905.55 | Joback Method |
| cpg | 887.40 | J/mol×K | 942.29 | Joback Method |
| cpg | 900.47 | J/mol×K | 979.04 | Joback Method |
| cpg | 912.34 | J/mol×K | 1015.78 | Joback Method |
| cpg | 923.04 | J/mol×K | 1052.53 | Joback Method |
| cpg | 932.62 | J/mol×K | 1089.27 | 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=U343845&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 |