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

**Inchi:** InChI=1S/C20H24O4/c1-6-23-19(21)16-8-7-9-17(13-16)20(22)24-18(12-15(4)5)11-10-14

**InchiKey:** DEPXDXHSFRILSA-UHFFFAOYSA-N

**Formula:** C20H24O4

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

**Mol. weight [g/mol]:** 328.40

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 29.67 | kJ/mol | Joback Method |
| hf | -343.29 | kJ/mol | Joback Method |
| hfus | 40.27 | kJ/mol | Joback Method |
| hvap | 82.15 | kJ/mol | Joback Method |
| log10ws | -5.66 | | Crippen Method |
| logp | 4.014 | | Crippen Method |
| mcvol | 270.880 | ml/mol | McGowan Method |
| pc | 1591.08 | kPa | Joback Method |
| rinpol | 2315.00 | | NIST Webbook |
| rinpol | 2315.00 | | NIST Webbook |
| tb | 845.92 | K | Joback Method |
| tc | 1068.08 | K | Joback Method |
| tf | 558.80 | K | Joback Method |
| vc | 1.028 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 799.48 | J/mol×K | 845.92 | Joback Method |
| cpg | 814.93 | J/mol×K | 882.95 | Joback Method |
| cpg | 829.15 | J/mol×K | 919.97 | Joback Method |
| cpg | 842.16 | J/mol×K | 957.00 | Joback Method |
| cpg | 853.99 | J/mol×K | 994.03 | Joback Method |
| cpg | 864.67 | J/mol×K | 1031.05 | Joback Method |
| cpg | 874.23 | J/mol×K | 1068.08 | 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=U343844&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 |