# Isophthalic acid, 3,7-dimethyloct-6-enyl propyl ester

**Inchi:** InChI=1S/C21H30O4/c1-5-13-24-20(22)18-10-7-11-19(15-18)21(23)25-14-12-17(4)9-6-8

**InchiKey:** WBWMGSFDLSWXCI-UHFFFAOYSA-N

**Formula:** C21H30O4

**SMILES:** CCCOC(=O)c1cccc(C(=O)OCCC(C)CCC=C(C)C)c1

**Mol. weight [g/mol]:** 346.46

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -169.89 | kJ/mol | Joback Method |
| hf | -639.16 | kJ/mol | Joback Method |
| hfus | 44.74 | kJ/mol | Joback Method |
| hvap | 83.24 | kJ/mol | Joback Method |
| log10ws | -6.17 | | Crippen Method |
| logp | 5.183 | | Crippen Method |
| mcvol | 293.570 | ml/mol | McGowan Method |
| pc | 1311.80 | kPa | Joback Method |
| rinpol | 2492.00 | | NIST Webbook |
| tb | 867.72 | K | Joback Method |
| tc | 1075.69 | K | Joback Method |
| tf | 475.65 | K | Joback Method |
| vc | 1.127 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 910.41 | J/mol×K | 867.72 | Joback Method |
| cpg | 926.54 | J/mol×K | 902.38 | Joback Method |
| cpg | 941.51 | J/mol×K | 937.04 | Joback Method |
| cpg | 955.37 | J/mol×K | 971.70 | Joback Method |
| cpg | 968.17 | J/mol×K | 1006.36 | Joback Method |
| cpg | 979.93 | J/mol×K | 1041.03 | Joback Method |
| cpg | 990.70 | J/mol×K | 1075.69 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U356736&Units=SI |
| **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 |

# Legend

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