# Isophthalic acid, hex-3-yl tetradecyl ester

**Inchi:** InChI=1S/C28H46O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-22-31-27(29)24-20-18-21-25(
**InchiKey:** PGRFLBUIGTVQQA-UHFFFAOYSA-N
**Formula:** C28H46O4
**SMILES:** CCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(CC)CCC)c1
**Mol. weight [g/mol]:** 446.66

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -182.62 | kJ/mol | Joback Method |
| hf | -891.07 | kJ/mol | Joback Method |
| hfus | 63.98 | kJ/mol | Joback Method |
| hvap | 98.78 | kJ/mol | Joback Method |
| log10ws | -9.60 | | Crippen Method |
| logp | 8.280 | | Crippen Method |
| mcvol | 396.500 | ml/mol | McGowan Method |
| pc | 821.01 | kPa | Joback Method |
| rinpol | 3244.00 | | NIST Webbook |
| tb | 1023.84 | K | Joback Method |
| tc | 1257.25 | K | Joback Method |
| tf | 573.58 | K | Joback Method |
| vc | 1.538 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1369.87 | J/mol×K | 1023.84 | Joback Method |
| cpg | 1443.15 | J/mol×K | 1218.35 | Joback Method |
| cpg | 1431.78 | J/mol×K | 1179.45 | Joback Method |
| cpg | 1418.83 | J/mol×K | 1140.55 | Joback Method |
| cpg | 1404.24 | J/mol×K | 1101.64 | Joback Method |
| cpg | 1387.95 | J/mol×K | 1062.74 | Joback Method |
| cpg | 1453.02 | J/mol×K | 1257.25 | Joback Method |
| dvisc | 0.0000152 | Pa×s | 1023.84 | Joback Method |
| dvisc | 0.0000203 | Pa×s | 948.80 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000283 | Pa×s | 873.75 | Joback Method |
| dvisc | 0.0000422 | Pa×s | 798.71 | Joback Method |
| dvisc | 0.0000682 | Pa×s | 723.67 | Joback Method |
| dvisc | 0.0001234 | Pa×s | 648.62 | Joback Method |
| dvisc | 0.0002604 | Pa×s | 573.58 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U356481&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

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

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