# Isophthalic acid, hept-3-yl hexadecyl ester

**Inchi:** InChI=1S/C31H52O4/c1-4-7-9-10-11-12-13-14-15-16-17-18-19-20-25-34-30(32)27-22-21
**InchiKey:** GGAFKXAWDCXGNF-UHFFFAOYSA-N
**Formula:** C31H52O4
**SMILES:** CCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(CC)CCCC)c1
**Mol. weight [g/mol]:** 488.74

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -157.36 | kJ/mol | Joback Method |
| hf | -952.99 | kJ/mol | Joback Method |
| hfus | 71.75 | kJ/mol | Joback Method |
| hvap | 105.46 | kJ/mol | Joback Method |
| log10ws | -10.86 | | Crippen Method |
| logp | 9.450 | | Crippen Method |
| mcvol | 438.770 | ml/mol | McGowan Method |
| pc | 700.61 | kPa | Joback Method |
| rinpol | 3429.00 | | NIST Webbook |
| tb | 1092.48 | K | Joback Method |
| tc | 1356.26 | K | Joback Method |
| tf | 607.39 | K | Joback Method |
| vc | 1.706 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1560.96 | J/mol×K | 1092.48 | Joback Method |
| cpg | 1580.15 | J/mol×K | 1136.44 | Joback Method |
| cpg | 1597.09 | J/mol×K | 1180.41 | Joback Method |
| cpg | 1611.87 | J/mol×K | 1224.37 | Joback Method |
| cpg | 1624.62 | J/mol×K | 1268.34 | Joback Method |
| cpg | 1635.46 | J/mol×K | 1312.30 | Joback Method |
| cpg | 1644.50 | J/mol×K | 1356.26 | Joback Method |
| dvisc | 0.0001743 | Pa×s | 607.39 | Joback Method |
| dvisc | 0.0000806 | Pa×s | 688.24 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000439 | Pa×s | 769.09 | Joback Method |
| dvisc | 0.0000268 | Pa×s | 849.93 | Joback Method |
| dvisc | 0.0000178 | Pa×s | 930.78 | Joback Method |
| dvisc | 0.0000127 | Pa×s | 1011.63 | Joback Method |
| dvisc | 0.0000095 | Pa×s | 1092.48 | Joback Method |

# Sources

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|---|---|
| **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=U356524&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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