# Isophthalic acid, 8-chloroctyl heptyl ester

**Inchi:** InChI=1S/C23H35ClO4/c1-2-3-4-8-11-17-27-22(25)20-14-13-15-21(19-20)23(26)28-18-1
**InchiKey:** JVYHSDDLTVVGCE-UHFFFAOYSA-N
**Formula:** C23H35ClO4
**SMILES:** CCCCCCCOC(=O)c1cccc(C(=O)OCCCCCCCCCl)c1
**Mol. weight [g/mol]:** 410.98

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -234.21 | kJ/mol | Joback Method |
| hf | -798.33 | kJ/mol | Joback Method |
| hfus | 58.75 | kJ/mol | Joback Method |
| hvap | 92.43 | kJ/mol | Joback Method |
| log10ws | -7.55 | | Crippen Method |
| logp | 6.550 | | Crippen Method |
| mcvol | 338.290 | ml/mol | McGowan Method |
| pc | 1071.46 | kPa | Joback Method |
| rinpol | 3086.00 | | NIST Webbook |
| tb | 947.31 | K | Joback Method |
| tc | 1160.48 | K | Joback Method |
| tf | 562.15 | K | Joback Method |
| vc | 1.312 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1084.97 | J/mol×K | 947.31 | Joback Method |
| cpg | 1100.59 | J/mol×K | 982.84 | Joback Method |
| cpg | 1114.89 | J/mol×K | 1018.37 | Joback Method |
| cpg | 1127.90 | J/mol×K | 1053.89 | Joback Method |
| cpg | 1139.65 | J/mol×K | 1089.42 | Joback Method |
| cpg | 1150.19 | J/mol×K | 1124.95 | Joback Method |
| cpg | 1159.55 | J/mol×K | 1160.48 | Joback Method |
| dvisc | 0.0003455 | Pa×s | 562.15 | Joback Method |
| dvisc | 0.0001870 | Pa×s | 626.34 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001135 | Pa×s | 690.54 | Joback Method |
| dvisc | 0.0000750 | Pa×s | 754.73 | Joback Method |
| dvisc | 0.0000529 | Pa×s | 818.92 | Joback Method |
| dvisc | 0.0000392 | Pa×s | 883.12 | Joback Method |
| dvisc | 0.0000303 | Pa×s | 947.31 | 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=U356391&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 |