# Isophthalic acid, monoamide, N-(2-chlorophenyl)-, octyl ester

**Inchi:** InChI=1S/C22H26ClNO3/c1-2-3-4-5-6-9-15-27-22(26)18-12-10-11-17(16-18)21(25)24-20

**InchiKey:** YETKWBVQCDLZOT-UHFFFAOYSA-N

**Formula:** C22H26ClNO3

**SMILES:** CCCCCCCCOC(=O)c1cccc(C(O)=Nc2ccccc2Cl)c1

**Mol. weight [g/mol]:** 387.90

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -387.63 | kJ/mol | Joback Method |
| hvap | 104.06 | kJ/mol | Joback Method |
| log10ws | -7.01 | | Crippen Method |
| logp | 6.494 | | Crippen Method |
| mcvol | 304.550 | ml/mol | McGowan Method |
| pc | 1374.80 | kPa | Joback Method |
| rinpol | 3270.00 | | NIST Webbook |
| rinpol | 3270.00 | | NIST Webbook |
| tb | 1048.54 | K | Joback Method |
| tc | 1285.83 | K | Joback Method |

## Sources

**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=U345822&Units=SI

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

## Legend

**hf:** Enthalpy of formation 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 |