# Isophthalic acid, monoamide, N-(3-methylphenyl)-, heptyl ester

**Inchi:** InChI=1S/C22H27NO3/c1-3-4-5-6-7-14-26-22(25)19-12-9-11-18(16-19)21(24)23-20-13-8

**InchiKey:** DULWEOAFDUOKGN-UHFFFAOYSA-N

**Formula:** C22H27NO3

**SMILES:** CCCCCCCOC(=O)c1cccc(C(O)=Nc2cccc(C)c2)c1

**Mol. weight [g/mol]:** 353.45

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -371.89 | kJ/mol | Joback Method |
| hvap | 99.67 | kJ/mol | Joback Method |
| log10ws | -6.39 | | Crippen Method |
| logp | 5.759 | | Crippen Method |
| mcvol | 292.310 | ml/mol | McGowan Method |
| pc | 1413.31 | kPa | Joback Method |
| rinpol | 3191.00 | | NIST Webbook |
| rinpol | 3191.00 | | NIST Webbook |
| tb | 1011.11 | K | Joback Method |
| tc | 1241.99 | K | Joback Method |

## Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U345792&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

**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 |