# Isonicotinamide, N,N-diheptyl-

**Inchi:** InChI=1S/C20H34N2O/c1-3-5-7-9-11-17-22(18-12-10-8-6-4-2)20(23)19-13-15-21-16-14-
**InchiKey:** NVRWTGYHNXQINS-UHFFFAOYSA-N
**Formula:** C20H34N2O
**SMILES:** CCCCCCCN(CCCCCCC)C(=O)c1ccncc1
**Mol. weight [g/mol]:** 318.50

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -6.40 | | Crippen Method |
| logp | 5.465 | | Crippen Method |
| mcvol | 290.430 | ml/mol | McGowan Method |
| rinpol | 2366.00 | | NIST Webbook |
| rinpol | 2366.00 | | NIST Webbook |

## Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U308643&Units=SI

## Legend

**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume
**rinpol:** Non-polar retention indices

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