

Isonipecotic acid, N-(octanoyl)-, hexyl ester

| | |
|-----------------------------|---|
| Inchi: | InChI=1S/C20H37NO3/c1-3-5-7-9-10-12-19(22)21-15-13-18(14-16-21)20(23)24-17-11-8 |
| InchiKey: | NUKBWYIGJCUIRY-UHFFFAOYSA-N |
| Formula: | C20H37NO3 |
| SMILES: | CCCCCCCC(=O)N1CCC(C(=O)OCCCCC)CC1 |
| Mol. weight [g/mol]: | 339.51 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -5.06 | | Crippen Method |
| logp | 4.709 | | Crippen Method |
| mcvol | 300.790 | ml/mol | McGowan Method |
| rinpola | 2662.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U361572&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.cheméo.com/doc/models/crippen_log10ws |

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/30-321-1/Isonipecotic-acid-N-octanoyl-hexyl-ester.pdf>

Generated by Cheméo on 2024-04-26 18:33:18.676557398 +0000 UTC m=+16445647.597134713.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.