

# Isonipecotic acid, N-(2-fluoro-3-trifluoromethylbenzoyl)-, hexyl ester

InChI: InChI=1S/C20H25F4NO3/c1-2-3-4-5-13-28-19(27)14-9-11-25(12-10-14)18(26)15-7-6-8-1  
InChIKey: PEOBFFWGLSQBHE-UHFFFAOYSA-N

Formula: C20H25F4NO3

SMILES: CCCCCCOC(=O)C1CCN(C(=O)c2cccc(C(F)(F)F)c2F)CC1

Mol. weight [g/mol]: 403.41

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -5.75   |        | Crippen Method |
| logp          | 4.820   |        | Crippen Method |
| mcvol         | 284.110 | ml/mol | McGowan Method |
| rinpol        | 2536.00 |        | NIST Webbook   |

## Sources

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

Crippen Method: [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=U361312&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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