Isonipecotic acid, N-(3-fluorobenzoyl)-, heptyl ester

Inchi: InChI=1S/C20H28FNO3/c1-2-3-4-5-6-14-25-20(24)16-10-12-22(13-11-16)19(23)17-8-7-9
InchiKey: YFTAZAIPCHGPCQ-UHFFFAOYSA-N
Formula: C20H28FNO3
SMILES: CCCCCCCOC(=O)C1CCN(C(=O)c2cccc(F)c2)CC1
Mol. weight [g/mol]: 349.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.07		Crippen Method
logp	4.191		Crippen Method
mcvol	278.800	ml/mol	McGowan Method
rinpol	2724.00		NIST Webbook
rinpol	2724.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361523&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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