Isonipecotic acid, N-(2-trifluoromethylbenzoyl)-, decyl ester

Inchi: InChI=1S/C24H34F3NO3/c1-2-3-4-5-6-7-8-11-18-31-23(30)19-14-16-28(17-15-19)22(29)
InchiKey: PTQVJPUSVFSEGC-UHFFFAOYSA-N
Formula: C24H34F3NO3
SMILES: CCCCCCCCCCOC(=O)C1CCN(C(=O)c2ccccc2C(F)(F)F)CC1
Mol. weight [g/mol]: 441.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.09		Crippen Method
logp	6.242		Crippen Method
mcvol	338.700	ml/mol	McGowan Method
rinpol	3005.00		NIST Webbook
rinpol	3005.00		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=U361495&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

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