Isonipecotic acid, N-(2,5-di(trifluoromethyl)benzoyl)-, undecyl ester

Inchi: InChI=1S/C26H35F6NO3/c1-2-3-4-5-6-7-8-9-10-17-36-24(35)19-13-15-33(16-14-19)23(3

InchiKey: AELXHBLKHCHVSF-UHFFFAOYSA-N

Formula: C26H35F6NO3

SMILES: CCCCCCCCCCCOC(=O)C1CCN(C(=O)c2cc(C(F)(F)F)ccc2C(F)(F)F)CC1

Mol. weight [g/mol]: 523.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.62		Crippen Method
logp	7.650		Crippen Method
mcvol	372.190	ml/mol	McGowan Method
rinpol	2852.00		NIST Webbook
rinpol	2852.00		NIST Webbook

Sources

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=U361211&Units=SI

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

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.