Isonipecotic acid, N-(3,4-difluorobenzoyl)-, butyl ester

Inchi: InChI=1S/C17H21F2NO3/c1-2-3-10-23-17(22)12-6-8-20(9-7-12)16(21)13-4-5-14(18)15(1

InchiKey: FFKOQXCGLOITMY-UHFFFAOYSA-N

Formula: C17H21F2NO3

SMILES: CCCCOC(=O)C1CCN(C(=O)c2ccc(F)c(F)c2)CC1

Mol. weight [g/mol]: 325.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.14		Crippen Method
logp	3.160		Crippen Method
mcvol	238.300	ml/mol	McGowan Method
rinpol	2400.00		NIST Webbook
rinpol	2400.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361265&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.