

Isonipecotinoylisonipecotic acid, N'-(2,4-difluorobenzoyl)-, propyl ester

Inchi:	InChI=1S/C22H28F2N2O4/c1-2-13-30-22(29)16-7-11-25(12-8-16)20(27)15-5-9-26(10-6-
InchiKey:	GRYSEGVTEOGHGI-UHFFFAOYSA-N
Formula:	C22H28F2N2O4
SMILES:	CCCOC(=O)C1CCN(C(=O)C2CCN(C(=O)c3ccc(F)cc3F)CC2)CC1
Mol. weight [g/mol]:	422.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.23		Crippen Method
logp	3.009		Crippen Method
mcvol	309.440	ml/mol	McGowan Method
rinsol	3433.00		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=U361383&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/40-405-7/Isonipecotinoylisonipecotic-acid-N-2-4-difluorobenzoyl-propyl-ester.pdf>

Generated by Cheméo on 2024-04-29 03:35:03.525165776 +0000 UTC m=+16650952.445743093.

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