

Isonipecotic acid, N-(2,6-difluoro-3-methylbenzoyl)-, propyl ester

Inchi: InChI=1S/C17H21F2NO3/c1-3-10-23-17(22)12-6-8-20(9-7-12)16(21)14-13(18)5-4-11(2)1
InchiKey: ZJLZTBQUXDXBIJ-UHFFFAOYSA-N
Formula: C17H21F2NO3
SMILES: CCCOC(=O)C1CCN(C(=O)c2c(F)ccc(C)c2F)CC1
Mol. weight [g/mol]: 325.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.20		Crippen Method
logp	3.079		Crippen Method
mcvol	238.300	ml/mol	McGowan Method
rinpol	2396.00		NIST Webbook
rinpol	2396.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361298&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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

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