

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

Inchi: InChI=1S/C16H19F2NO3/c1-3-22-16(21)11-6-8-19(9-7-11)15(20)13-12(17)5-4-10(2)14(1)
InchiKey: FHTXNKJQWHTWLD-UHFFFAOYSA-N
Formula: C16H19F2NO3
SMILES: CCOC(=O)C1CCN(C(=O)c2c(F)ccc(C)c2F)CC1
Mol. weight [g/mol]: 311.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.78		Crippen Method
logp	2.689		Crippen Method
mcvol	224.210	ml/mol	McGowan Method
rinpole	2292.00		NIST Webbook
rinpole	2292.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361297&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
rinpole: Non-polar retention indices

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