

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

Inchi: InChI=1S/C20H27F2NO3/c1-3-4-5-6-13-26-20(25)15-9-11-23(12-10-15)19(24)17-16(21)
InchiKey: GJQXZBHHJURJQF-UHFFFAOYSA-N
Formula: C20H27F2NO3
SMILES: CCCCCOC(=O)C1CCN(C(=O)c2c(F)ccc(C)c2F)CC1
Mol. weight [g/mol]: 367.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.46		Crippen Method
logp	4.249		Crippen Method
mcvol	280.570	ml/mol	McGowan Method
rinpola	2706.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361303&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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
rinpola: Non-polar retention indices

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