

Isonipecotic acid, N-(2,5-difluorobenzoyl)-, butyl ester

Inchi: InChI=1S/C17H21F2NO3/c1-2-3-10-23-17(22)12-6-8-20(9-7-12)16(21)14-11-13(18)4-5-1
InchiKey: NRJXPCOGYLMDAG-UHFFFAOYSA-N
Formula: C17H21F2NO3
SMILES: CCCCOC(=O)C1CCN(C(=O)c2cc(F)ccc2F)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
rinpola	2368.00		NIST Webbook
rinpola	2368.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361411&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
rinpola: Non-polar retention indices

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