L-Proline, N-(2,6-difluorobenzoyl)-, methyl ester

Inchi: InChI=1S/C13H13F2NO3/c1-19-13(18)10-6-3-7-16(10)12(17)11-8(14)4-2-5-9(11)15/h2,4

InchiKey: QVKVHEIVKOWIQQ-UHFFFAOYSA-N

Formula: C13H13F2NO3

SMILES: COC(=O)C1CCCN1C(=O)c1c(F)cccc1F

Mol. weight [g/mol]: 269.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.91		Cheméo Relay (1.0)
logp	1.742		Crippen Method
mcvol	181.940	ml/mol	McGowan Method
rinpol	1840.00		NIST Webbook
tf	346.44	K	Cheméo Relay (1.0)

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299662&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

tf: Normal melting (fusion) point