

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

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