L-Proline, N-(3,4-difluorobenzoyl)-, butyl ester

Inchi: InChI=1S/C16H19F2NO3/c1-2-3-9-22-16(21)14-5-4-8-19(14)15(20)11-6-7-12(17)13(18)1
InchiKey: XJQILOBNQWOLDB-UHFFFAOYSA-N
Formula: C16H19F2NO3
SMILES: CCCCOC(=O)C1CCCN1C(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 311.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.08		Crippen Method
logp	2.913		Crippen Method
mcvol	224.210	ml/mol	McGowan Method
rinpol	2171.00		NIST Webbook
rinpol	2171.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U345910&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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