L-Proline, N-(2,6-difluoro-3-methylbenzoyl)-, isobutyl ester

Inchi: InChI=1S/C17H21F2NO3/c1-10(2)9-23-17(22)13-5-4-8-20(13)16(21)14-12(18)7-6-11(3)1

InchiKey: LJADLFDCNSFJRF-UHFFFAOYSA-N

Formula: C17H21F2NO3

SMILES: Cc1ccc(F)c(C(=O)N2CCCC2C(=O)OCC(C)C)c1F

Mol. weight [g/mol]: 325.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.31		Crippen Method
logp	3.077		Crippen Method
mcvol	238.300	ml/mol	McGowan Method
rinpol	2240.00		NIST Webbook
rinpol	2240.00		NIST Webbook

Sources

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

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=U345886&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.