

Isonipectinoylisonipectic acid, N'-pentafluorobenzoyl-, propyl ester

Inchi: InChI=1S/C22H25F5N2O4/c1-2-11-33-22(32)13-5-9-28(10-6-13)20(30)12-3-7-29(8-4-12)
InchiKey: YMRRYQDDUNQWNJ-UHFFFAOYSA-N
Formula: C22H25F5N2O4
SMILES: CCCOC(=O)C1CCN(C(=O)C2CCN(C(=O)c3c(F)c(F)c(F)c(F)c3F)CC2)CC1
Mol. weight [g/mol]: 476.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.23		Crippen Method
logp	3.426		Crippen Method
mcvol	314.750	ml/mol	McGowan Method
rinpol	3247.00		NIST Webbook
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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=U361234&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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