L-Proline, N-(pentafluorobenzoyl)-, octyl ester

Inchi: InChI=1S/C20H24F5NO3/c1-2-3-4-5-6-7-11-29-20(28)12-9-8-10-26(12)19(27)13-14(21)1
InchiKey: HCUWTCVZFRZQFR-UHFFFAOYSA-N
Formula: C20H24F5NO3
SMILES: CCCCCCCCOC(=O)C1CCCN1C(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 421.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.75		Crippen Method
logp	4.890		Crippen Method
mcvol	285.880	ml/mol	McGowan Method
rinpol	2385.00		NIST Webbook
rinpol	2385.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346298&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.