

Isonipecotic acid, N-pentafluorobenzoyl-, pentyl ester

Inchi: InChI=1S/C18H20F5NO3/c1-2-3-4-9-27-18(26)10-5-7-24(8-6-10)17(25)11-12(19)14(21)1
InchiKey: FOJCQQHBIIRSIG-UHFFFAOYSA-N
Formula: C18H20F5NO3
SMILES: CCCCCOC(=O)C1CCN(C(=O)c2c(F)c(F)c(F)c(F)c2F)CC1
Mol. weight [g/mol]: 393.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.56		Crippen Method
logp	3.968		Crippen Method
mcvol	257.700	ml/mol	McGowan Method
rinpola	2307.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361224&Units=SI>
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>

Legend

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

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