

Isonipecotic acid, N-pentafluorobenzoyl-, heptyl ester

Inchi: InChI=1S/C20H24F5NO3/c1-2-3-4-5-6-11-29-20(28)12-7-9-26(10-8-12)19(27)13-14(21)1
InchiKey: MIVKPNGPUKLFKW-UHFFFAOYSA-N
Formula: C20H24F5NO3
SMILES: CCCCCCOC(=O)C1CCN(C(=O)c2c(F)c(F)c(F)c(F)c2F)CC1
Mol. weight [g/mol]: 421.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.39		Crippen Method
logp	4.748		Crippen Method
mcvol	285.880	ml/mol	McGowan Method
rinpola	2506.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U361227&Units=SI>

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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