

Isonipecotic acid, N-pentafluorobenzoyl-, ethyl ester

Inchi: InChI=1S/C15H14F5NO3/c1-2-24-15(23)7-3-5-21(6-4-7)14(22)8-9(16)11(18)13(20)12(19)
InchiKey: UNCLJTXXIGBVMY-UHFFFAOYSA-N
Formula: C15H14F5NO3
SMILES: CCOC(=O)C1CCN(C(=O)c2c(F)c(F)c(F)c(F)c2F)CC1
Mol. weight [g/mol]: 351.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.30		Crippen Method
logp	2.797		Crippen Method
mcvol	215.430	ml/mol	McGowan Method
rinpol	2004.00		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=U361220&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

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