

Isonipecotic acid, N-(2,5-di(trifluoromethyl)benzoyl)-, pentyl ester

InChI: InChI=1S/C20H23F6NO3/c1-2-3-4-11-30-18(29)13-7-9-27(10-8-13)17(28)15-12-14(19(20)16)5-6
InChIKey: XNRGFGFSXRPKQJ-UHFFFAOYSA-N
Formula: C20H23F6NO3
SMILES: CCCCCOC(=O)C1CCN(C(=O)c2cc(C(F)(F)F)ccc2C(F)(F)F)CC1
Mol. weight [g/mol]: 439.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.11		Crippen Method
logp	5.310		Crippen Method
mcvol	287.650	ml/mol	McGowan Method
rinpol	2277.00		NIST Webbook
rinpol	2277.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=U361204&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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