

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

Inchi: InChI=1S/C19H21F6NO3/c1-2-3-10-29-17(28)12-6-8-26(9-7-12)16(27)14-11-13(18(20,21)19)/m 1
InchiKey: SAWNNFPCXSHENA-UHFFFAOYSA-N
Formula: C19H21F6NO3
SMILES: CCCCO(=O)C1CCN(C(=O)c2cc(C(F)(F)F)ccc2C(F)(F)F)CC1
Mol. weight [g/mol]: 425.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.69		Crippen Method
logp	4.920		Crippen Method
mcvol	273.560	ml/mol	McGowan Method
rinpole	2176.00		NIST Webbook
rinpole	2176.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361203&Units=SI>
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>

Legend

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

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