

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

Inchi: InChI=1S/C21H25F6NO3/c1-2-3-4-5-12-31-19(30)14-8-10-28(11-9-14)18(29)16-13-15(20)
InchiKey: MFPYFAILRPHXBC-UHFFFAOYSA-N
Formula: C₂₁H₂₅F₆NO₃
SMILES: CCCCCOC(=O)C1CCN(C(=O)c2cc(C(F)(F)F)ccc2C(F)(F)F)CC1
Mol. weight [g/mol]: 453.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.52		Crippen Method
logp	5.700		Crippen Method
mcvol	301.740	ml/mol	McGowan Method
rinpol	2374.00		NIST Webbook
rinpol	2374.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361206&Units=SI>
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>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/113-501-9/Isonipecotic-acid-N-2-5-di-trifluoromethyl-benzoyl-hexyl-ester.pdf>

Generated by Cheméo on 2024-04-29 04:21:53.88784144 +0000 UTC m=+16653762.808418752.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.