

3-Trifluoroacetyloxybenzoic acid, 3-(trimethylsilyloxycarbonyl)phenyl ester

Inchi: InChI=1S/C19H17F3O6Si/c1-29(2,3)28-17(24)13-7-5-8-14(11-13)26-16(23)12-6-4-9-15(1)
InchiKey: OHZJAIZULNFHTO-UHFFFAOYSA-N
Formula: C19H17F3O6Si
SMILES: C[Si](C)(C)OC(=O)c1cccc(OC(=O)c2cccc(OC(=O)C(F)(F)F)c2)c1
Mol. weight [g/mol]: 426.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.67		Crippen Method
logp	4.365		Crippen Method
rinpol	2281.00		NIST Webbook
rinpol	2281.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375019&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/112-945-8/3-Trifluoroacetyloxybenzoic-acid-3-trimethylsilyloxycarbonyl-phenyl-ester.pdf>

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