

Anthranilic acid, N-trifluoroacetyl-, trimethylsilyl ester

Inchi: InChI=1S/C12H14F3NO3Si/c1-20(2,3)19-10(17)8-6-4-5-7-9(8)16-11(18)12(13,14)15/h4-7
InchiKey: AOIBALIHOKJKLI-UHFFFAOYSA-N
Formula: C12H14F3NO3Si
SMILES: C[Si](C)(C)OC(=O)c1ccccc1NC(=O)C(F)(F)F
Mol. weight [g/mol]: 305.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.47		Crippen Method
logp	3.179		Crippen Method
rinpol	1520.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375135&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/36-688-9/Anthranilic-acid-N-trifluoroacetyl-trimethylsilyl-ester.pdf>

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