

Anthranilic acid, N-heptafluorobutyryl-, trimethylsilyl ester

Inchi: InChI=1S/C14H14F7NO3Si/c1-26(2,3)25-10(23)8-6-4-5-7-9(8)22-11(24)12(15,16)13(17,18)14
InchiKey: OPXYAOKIXNLWKC-UHFFFAOYSA-N
Formula: C14H14F7NO3Si
SMILES: C[Si](C)(C)OC(=O)c1ccccc1NC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 405.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.93		Crippen Method
logp	4.450		Crippen Method
rinpol	1531.00		NIST Webbook
rinpol	1531.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375144&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/115-689-0/Anthranilic-acid-N-heptafluorobutyryl-trimethylsilyl-ester.pdf>

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