

4-Aminobenzoic acid, N,N-bis(pentafluoropropionyl)-, trimethylsilyl ester

InChI: InChI=1S/C16H13F10NO4Si/c1-32(2,3)31-10(28)8-4-6-9(7-5-8)27(11(29)13(17,18)15(21

InChIKey: GBNJGMIGACLWOP-UHFFFAOYSA-N

Formula: C16H13F10NO4Si

SMILES: C[Si](C)(C)OC(=O)c1ccc(N(C(=O)C(F)(F)C(F)(F)F)C(=O)C(F)(F)C(F)(F)F)cc1

Mol. weight [g/mol]: 501.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.69		Crippen Method
logp	4.933		Crippen Method
rinpol	1444.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375127&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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