

2-Aminobenzoic acid, N-pentafluoropropionyl-, tert.-butyldimethylsilyl ester

InChI: InChI=1S/C16H20F5NO3Si/c1-11(2,3)26(4,5)25-12(23)10-8-6-7-9-11(10)22-13(24)15(17)16
InChIKey: QKYAJZIOBKRVRI-UHFFFAOYSA-N

Formula: C16H20F5NO3Si
SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1ccccc1NC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 397.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.46		Crippen Method
logp	4.985		Crippen Method
rinpol	1725.00		NIST Webbook
rinpol	1725.00		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=U375102&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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