

4-Aminobenzoic acid, N- pentafluoropropionyl-, N,O-bis(tert.-butyldimethylsilyl)-

Inchi: InChI=1S/C22H34F5NO3Si2/c1-19(2,3)32(7,8)28(18(30)21(23,24)22(25,26)27)16-13-11
InchiKey: QIFADIKEQFILIO-UHFFFAOYSA-N
Formula: C22H34F5NO3Si2
SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1ccc(N(C(=O)C(F)(F)C(F)(F)F)[Si](C)(C)C(C)(C)C)cc1
Mol. weight [g/mol]: 511.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.50		Crippen Method
logp	7.384		Crippen Method
rinpol	2097.00		NIST Webbook
rinpol	2097.00		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=U375090&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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