

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

Inchi: InChI=1S/C23H34F7NO3Si2/c1-19(2,3)35(7,8)31(18(33)21(24,25)22(26,27)23(28,29)30)
InchiKey: DEWYOWADWVTSKP-UHFFFAOYSA-N
Formula: C23H34F7NO3Si2
SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1ccc(N(C(=O)C(F)(F)C(F)(F)C(F)(F)F)[Si](C)(C)C(C)(C)C)cc1
Mol. weight [g/mol]: 561.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.23		Crippen Method
logp	8.020		Crippen Method
rinpol	2106.00		NIST Webbook
rinpol	2106.00		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=U375088&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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