

Benzoic acid, 4-[(trimethylsilyl)amino]-, trimethylsilyl ester

Other names:

Benzoic acid, p-[(trimethylsilyl)amino]-, trimethylsilyl ester

p-Aminobenzoic acid (tms)

4-Aminobenzoic acid, TMS

Benzoic acid, 4-amino, TMS

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

Trimethylsilyl 4-[(trimethylsilyl)amino]benzoate

4-Aminobenzoic acid, 2tms derivative

Inchi:

InChI=1S/C13H23NO2Si2/c1-17(2,3)14-12-9-7-11(8-10-12)13(15)16-18(4,5)6/h7-10,14H

InchiKey:

UNEXFOGMEVUYSY-UHFFFAOYSA-N

Formula:

C13H23NO2Si2

SMILES:

C[Si](C)(C)Nc1ccc(C(=O)O[Si](C)(C)C)cc1

Mol. weight [g/mol]:

281.50

CAS:

18406-05-8

Physical Properties

Property code	Value	Unit	Source
log10ws	0.50		Crippen Method
logp	3.925		Crippen Method
rinqol	1836.00		NIST Webbook
rinqol	1813.00		NIST Webbook
rinqol	1848.00		NIST Webbook
rinqol	1836.00		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=C18406058&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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