

Benzoic acid, 2-[(trimethylsilyl)amino]-, trimethylsilyl ester

Other names:

Anthranilic acid, N-(trimethylsilyl)-, trimethylsilyl ester

Trimethylsilyl 2-[(trimethylsilyl)amino]benzoate

Benzoic acid, 2-amino, bis-TMS

Benzoic acid, 2-amino, TMS

Anthranilic acid, 2TMS

Anthranilic acid, 2tms derivative

Inchi:

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

InchiKey:

IQRKGLWGOYKGPT-UHFFFAOYSA-N

Formula:

C13H23NO2Si2

SMILES:

C[Si](C)(C)Nc1cccc1C(=O)O[Si](C)(C)C

Mol. weight [g/mol]:

281.50

CAS:

18406-07-0

Physical Properties

Property code	Value	Unit	Source
log10ws	0.50		Crippen Method
logp	3.925		Crippen Method
rinpol	1600.00		NIST Webbook
rinpol	1618.00		NIST Webbook
rinpol	1605.20		NIST Webbook
rinpol	1609.00		NIST Webbook
rinpol	1618.00		NIST Webbook
rinpol	1609.00		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=C18406070&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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