

Trimethylsilyl 2-[(4-aminobenzoyl)amino]acetate

Other names:

4-Aminohippuric acid, trimethylsilyl ester

Hippuric acid, p-amino-, trimethylsilyl ester

para-Aminohippuric acid, trimethylsilyl ester

Inchi: InChI=1S/C12H18N2O3Si/c1-18(2,3)17-11(15)8-14-12(16)9-4-6-10(13)7-5-9/h4-7H,8,13

InchiKey: KHCVEJYAKDIGEY-UHFFFAOYSA-N

Formula: C12H18N2O3Si

SMILES: C[Si](C)(C)OC(=O)CNC(=O)c1ccc(N)cc1

Mol. weight [g/mol]: 266.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.04		Crippen Method
logp	1.377		Crippen Method
rinpol	2374.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U373093&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/67-394-1/Trimethylsilyl-2-4-aminobenzoyl-amino-acetate.pdf>

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