

4-Bromophenoxyacetic acid, trimethylsilyl ester

Other names:	4-Bromophenoxyacetic acid, tms derivative
Inchi:	InChI=1S/C11H15BrO3Si/c1-16(2,3)15-11(13)8-14-10-6-4-9(12)5-7-10/h4-7H,8H2,1-3H3
InchiKey:	ILLFIXLGYJSDJJ-UHFFFAOYSA-N
Formula:	C11H15BrO3Si
SMILES:	C[Si](C)(C)OC(=O)COc1ccc(Br)cc1
Mol. weight [g/mol]:	303.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.34		Crippen Method
logp	3.206		Crippen Method
rinpol	1712.00		NIST Webbook
rinpol	1712.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333869&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/55-036-1/4-Bromophenoxyacetic-acid-trimethylsilyl-ester.pdf>

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