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
ie	8.36	eV	Cheméo Relay (1.0)
logp	3.206		Crippen Method
rinpol	1712.00		NIST Webbook
rinpol	1712.00		NIST Webbook
tb	580.26	K	Cheméo Relay (1.0)

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U333869&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie: Ionization energy
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature

Latest version available from:

https://www.chemeo.com/cid/55-036-1/4-Bromophenoxyacetic-acid-trimethylsilyl-ester.pdf

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