Trimethylsilyl 4-nitrobenzoate

Other names:	4-Nitrobenzoic acid, trimethylsilyl ester
Inchi:	InChI=1S/C10H13NO4Si/c1-16(2,3)15-10(12)8-4-6-9(7-5-8)11(13)14/h4-7H,1-3H3
InchiKey:	XWDMNLMNKPTAHM-UHFFFAOYSA-N
Formula:	C10H13NO4Si
SMILES:	C[Si](C)(C)OC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	239.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.25		Crippen Method
logp	2.587		Crippen Method
rinpol	1617.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373278&Units=SI

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/43-283-0/Trimethylsilyl-4-nitrobenzoate.pdf
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