3,5-Dinitrobenzyl alcohol, bromomethyldimethylsilyl ether

Inchi:	InChI=1S/C10H13BrN2O5Si/c1-19(2,7-11)18-6-8-3-9(12(14)15)5-10(4-8)13(16)17/h3-5H
InchiKey:	BADFRESYTLFJOF-UHFFFAOYSA-N
Formula:	C10H13BrN2O5Si
SMILES:	C[Si](C)(CBr)OCc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]:	349.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.57		Crippen Method
logp	3.159		Crippen Method
rinpol	2266.00		NIST Webbook
rinpol	2266.00		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=U376141&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/26-199-3/3-5-Dinitrobenzyl-alcohol-bromomethyldimethylsilyl-ether.pdf
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