3,5-Dinitrobenzyl alcohol, benzyldimethylsilyl ether

Inchi: InChI=1S/C16H18N2O5Si/c1-24(2,12-13-6-4-3-5-7-13)23-11-14-8-15(17(19)20)10-16(9-1

InchiKey: HBTOAUWRLJJLSL-UHFFFAOYSA-N

Formula: C16H18N2O5Si

SMILES: C[Si](C)(Cc1ccccc1)OCc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1

Mol. weight [g/mol]: 346.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.75		Crippen Method
logp	4.007		Crippen Method
rinpol	2556.00		NIST Webbook
rinpol	2556.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U376142&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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