1-(3-Cyanopropyl)dimethylsilyloxy-4-nitrobenzene

Inchi: InChI=1S/C12H16N2O3Si/c1-18(2,10-4-3-9-13)17-12-7-5-11(6-8-12)14(15)16/h5-8H,3-4
InchiKey: PJGVRRQPRCQLMW-UHFFFAOYSA-N
Formula: C12H16N2O3Si
SMILES: C[Si](C)(CCCC#N)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 264.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.25		Crippen Method
logp	3.482		Crippen Method
rinpol	2098.00		NIST Webbook
rinpol	2098.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U307934&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices