4-Fluoro-3-nitrobenzyl alcohol, (3-cyanopropyl)dimethylsilyl ether

Inchi: InChI=1S/C13H17FN2O3Si/c1-20(2,8-4-3-7-15)19-10-11-5-6-12(14)13(9-11)16(17)18/h5

InchiKey: OMMVQIXLFXGCBL-UHFFFAOYSA-N

Formula: C13H17FN2O3Si

SMILES: C[Si](C)(CCCC#N)OCc1ccc(F)c([N+](=O)[O-])c1

Mol. weight [g/mol]: 296.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.85		Crippen Method
logp	3.759		Crippen Method
rinpol	2181.00		NIST Webbook
rinpol	2181.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U376140&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