

4-Nitro-1-tributylsilyloxybenzene

Inchi: InChI=1S/C18H31NO3Si/c1-4-7-14-23(15-8-5-2,16-9-6-3)22-18-12-10-17(11-13-18)19(20-21)3
InchiKey: IWEKQSPCUZWGGC-UHFFFAOYSA-N
Formula: C18H31NO3Si
SMILES: CCCC[Si](CCCC)(CCCC)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 337.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.90		Crippen Method
logp	6.319		Crippen Method
rinpol	2286.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U307837&Units=SI>

Legend

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

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