4-Nitro-N-(4-p-tolyl-thiazol-2-yl)-benzeneamine, N-tert.-butyldimethylsilyl-

Inchi:	InChI=1S/C22H27N3O2SSi/c1-16-7-9-17(10-8-16)20-15-28-21(23-20)24(29(5,6)22(2,3)4
InchiKey:	PQHBJECBUMIGED-UHFFFAOYSA-N
Formula:	C22H27N3O2SSi
SMILES:	Cc1ccc(-c2csc(N(c3ccc([N+](=O)[O-])cc3)[Si](C)(C)C(C)(C)C)n2)cc1
Mol. weight [g/mol]:	425.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.57		Crippen Method
logp	7.170		Crippen Method
rinpol	3003.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374830&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

Latest version available from:
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