

7-Chloro-N-(3-[(diethylamino)methyl]-4-[(trimethylsilyl)oxy]phenyl)-N-(trimethylsilyl)quinoline

Other names: Phenol, 4-((7-chloro-4-quinoliny)trimethylsilylamino)-2-((diethylamino)methyl)-O-trimethylsilyl-Quinoline, 7-chloro-4-[[3-[(diethylamino)methyl]-4-dimethylsilyloxyphenyl]trimethylsilylamino]-4-[(7-chloro-4-quinolyl)trimethylsilylamino]-2-(diethylaminomethyl)phenol, trimethylsilyl ether, 7-Chloro-N-{3-[(diethylamino)methyl]-4-[(trimethylsilyl)oxy]phenyl}-N-(trimethylsilyl)quinoline

Inchi: InChI=1S/C26H38ClN3OSi2/c1-9-29(10-2)19-20-17-22(12-14-26(20)31-33(6,7)8)30(32(33)34)/p1

InchiKey: CUTKUZMEURZVHP-UHFFFAOYSA-N

Formula: C26H38ClN3OSi2

SMILES: CCN(CC)Cc1cc(N(c2ccnc3cc(Cl)ccc23)[Si](C)(C)C)ccc1O[Si](C)(C)C

Mol. weight [g/mol]: 500.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.45		Crippen Method
logp	7.917		Crippen Method
rinpol	2944.00		NIST Webbook

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U373436&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

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.