

Inabenfide, N,O-bis(tert-butyl dimethylsilyl)-

Inchi: InChI=1S/C31H43ClN2O2Si2/c1-30(2,3)37(7,8)34(29(35)24-18-20-33-21-19-24)27-17-16
InchiKey: MPAOOAFVPSEZOF-UHFFFAOYSA-N
Formula: C31H43ClN2O2Si2
SMILES: CC(C)(C)[Si](C)(C)OC(c1ccccc1)c1cc(Cl)ccc1N(C(=O)c1ccncc1)[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 567.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.15		Crippen Method
logp	9.498		Crippen Method
rinpol	3089.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U334044&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/30-862-1/Inabenfide-N-O-bis-tert-butyl dimethylsilyl.pdf>

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