2-(1-Naphthyl-N-trimethylsilyl-carbamoyl)benzoic acid, trimethylsilyl ester

Other names: 2-[(1-Naphthalenyl-N-trimethylsilylamino)carbonyl] benzoic Acid, trimethylsilyl ester
2-(1-Naphthylcarbamoyl)benzoic acid, 2TMS

Inchi: InChI=1S/C24H29NO3Si2/c1-29(2,3)25(22-17-11-13-18-12-7-8-14-19(18)22)23(26)20-15

InchiKey: CAVAVTFJURSCMM-UHFFFAOYSA-N

Formula: C24H29NO3Si2

SMILES: C[Si](C)(C)OC(=O)c1ccccc1C(=O)N(c1cccc2ccccc12)[Si](C)(C)C

Mol. weight [g/mol]: 435.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.17		Crippen Method
logp	6.313		Crippen Method
rinpol	2575.00		NIST Webbook
rinpol	2575.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373350&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices