2-Quinolinecarboxylic acid, 4-[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names: Kynurenic acid (2TMS)
Kynurenic acid di-TMS
Trimethylsilyl 4-[(trimethylsilyl)oxy]-2-quinolinecarboxylate
Kynurenic acid, trimethylsilyl ether, trimethylsilyl ester
Kinurenic acid, bis-TMS
Kynurenic acid, TMS
Kynurenic acid, 2tms derivative

Inchi: InChI=1S/C16H23NO3Si2/c1-21(2,3)19-15-11-14(16(18)20-22(4,5)6)17-13-10-8-7-9-12(1

InchiKey: UWPAYSHAYKTMBD-UHFFFAOYSA-N

Formula: C16H23NO3Si2

SMILES: C[Si](C)(C)OC(=O)c1cc(O[Si](C)(C)C)c2ccccc2n1

Mol. weight [g/mol]: 333.53

CAS: 36972-84-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.18		Crippen Method
logp	4.440		Crippen Method
rinpol	2093.00		NIST Webbook
rinpol	2059.00		NIST Webbook
rinpol	2078.80		NIST Webbook

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C36972846&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices