

2-Quinolinecarboxylic acid, 4,8-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names:
ester

Xanthurenic acid, O,O-bis(trimethylsilyl)-, trimethylsilyl ester

Xanthurenic acid, tris-TMS

Xanthurenic acid, TMS

Xanthurenic acid, 3tms derivative

Inchi: InChI=1S/C19H31NO4Si3/c1-25(2,3)22-16-12-10-11-14-17(23-26(4,5)6)13-15(20-18(14)

InchiKey: YLJWZSLESGYQOM-UHFFFAOYSA-N

Formula: C19H31NO4Si3

SMILES: C[Si](C)(C)OC(=O)c1cc(O[Si](C)(C)C)c2cccc(O[Si](C)(C)C)c2n1

Mol. weight [g/mol]: 421.71

CAS: 55319-89-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.19		Crippen Method
logp	5.654		Crippen Method
rinsol	2265.00		NIST Webbook
rinsol	2254.70		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C55319896&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinsol: Non-polar retention indices

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