3,5-BIS(TRIMETHYLSILOXY)BENZOIC ACID, TRIMETHYLSILYL ESTER

Other names: 3,5-Dihydroxybenzoic acid, bis(trimethylsilyl) ether, trimethylsilyl ester
Benzoic acid, 3,5-bis-(trimethylsilyloxy), trimethylsilyl ester
Benzoic acid, 3,5-dihydroxy, tris-TMS
Benzoic acid, 3,5-dihydroxy, TMS
Trimethylsilyl 3,5-bis[(trimethylsilyl)oxy]benzoate
3,5-Dihydroxybenzoic acid, 3tms derivative

Inchi: InChI=1S/C16H30O4Si3/c1-21(2,3)18-14-10-13(16(17)20-23(7,8)9)11-15(12-14)19-22(4,

InchiKey: ASTWSDQOZSFLPZ-UHFFFAOYSA-N

Formula: C16H30O4Si3

SMILES: C[Si](C)(C)OC(=O)c1cc(O[Si](C)(C)C)cc(O[Si](C)(C)C)c1

Mol. weight [g/mol]: 370.67

Physical Properties

Property code	Value	Unit	Source
logp	5.106		Crippen Method
rinpol	1828.00		NIST Webbook
rinpol	1830.00		NIST Webbook
rinpol	1803.20		NIST Webbook
rinpol	1828.00		NIST Webbook
tb	583.04	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C79314275&Units=SI

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

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

Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

tb: Normal Boiling Point Temperature