

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]: 370.66

CAS: 79314-27-5

Physical Properties

Property code	Value	Unit	Source
log10ws	1.38		Crippen Method
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

Sources

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

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

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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