

Benzoic acid, 3,4-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names:

Trimethylsilyl 3,4-bis(trimethylsilyloxy)benzoate

Protocatechuic acid (tms)

Benzoic acid, 3,4-dihydroxy, TMS

Protocatechuic acid, di-TMS

Protocatechuic acid, 3tms derivative

Inchi: InChI=1S/C16H30O4Si3/c1-21(2,3)18-14-11-10-13(16(17)20-23(7,8)9)12-15(14)19-22(4,5)

InchiKey: DVAGRNBURDZPDF-UHFFFAOYSA-N

Formula: C16H30O4Si3

SMILES: C[Si](C)(C)OC(=O)c1ccc(O[Si](C)(C)C)c(O[Si](C)(C)C)c1

Mol. weight [g/mol]: 370.66

CAS: 2347-40-2

Physical Properties

Property code	Value	Unit	Source
log10ws	1.38		Crippen Method
logp	5.106		Crippen Method
rinpol	1844.00		NIST Webbook
rinpol	1835.00		NIST Webbook
rinpol	1844.00		NIST Webbook
rinpol	1826.00		NIST Webbook
rinpol	1826.00		NIST Webbook
rinpol	1828.00		NIST Webbook
rinpol	1813.20		NIST Webbook
rinpol	1826.00		NIST Webbook
rinpol	1836.00		NIST Webbook
rinpol	1828.00		NIST Webbook
rinpol	1832.00		NIST Webbook
rinpol	1835.00		NIST Webbook
rinpol	1835.00		NIST Webbook
rinpol	1836.00		NIST Webbook
rinpol	1826.00		NIST Webbook
rinpol	1813.20		NIST Webbook
rinpol	1834.00		NIST Webbook
rinpol	1835.00		NIST Webbook
rinpol	1834.00		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=C2347402&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/119-527-5/Benzoic-acid-3-4-bis-trimethylsilyl-oxy-trimethylsilyl-ester.pdf>

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