

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

Other names:

«beta»-Resorcylic acid (TMS)
2,4-Bis(trimethylsiloxy)trimethylsilylbenzoate
2,4-Dihydroxybenzoic acid, bis(trimethylsilyl) ether, trimethylsilyl ester
2-Resorcylic acid, tri-TMS
Benzoic acid, 2,4-dihydroxy, TMS
Trimethylsilyl 2,4-bis[(trimethylsilyl)oxy]benzoate
2,4-Dihydroxybenzoic acid, 3tms derivative

Inchi:

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

InchiKey:

VOVIHULKTBZND-UHFFFAOYSA-N

Formula:

C16H30O4Si3

SMILES:

C[Si](C)(C)OC(=O)c1ccc(O[Si](C)(C)C)cc1O[Si](C)(C)C

Mol. weight [g/mol]:

370.66

CAS:

10586-16-0

Physical Properties

Property code	Value	Unit	Source
log10ws	1.38		Crippen Method
logp	5.106		Crippen Method
rinpol	1832.00		NIST Webbook
rinpol	1822.00		NIST Webbook
rinpol	1818.00		NIST Webbook
rinpol	1822.00		NIST Webbook
rinpol	1832.00		NIST Webbook
rinpol	1825.00		NIST Webbook
rinpol	1800.30		NIST Webbook
ripol	1637.00		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=C10586160&Units=SI>

Legend

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

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