

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

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