

Benzoic acid, 2,5-bis(trimethylsiloxy)-, trimethylsilyl ester

Other names:

Gentisic acid (tms)
Benzoic acid, 2,5-bis-(trimethylsilyloxy), trimethylsilyl ester
Benzoic acid, 2,5-dihydroxy, tri-TMS
Gentisic acid, O,O'-bis(trimethylsilyl)-, trimethylsilyl ester
Gentisic acid, tri-TMS
Benzoic acid, 2,5-dihydroxy, TMS
Gentisic acid, di-TMS
2,5-Dihydroxybenzoic acid, 3tms derivative

Inchi:

InChI=1S/C16H30O4Si3/c1-21(2,3)18-13-10-11-15(19-22(4,5)6)14(12-13)16(17)20-23(7,

InchiKey:

UBHIYVHURJXNOQ-UHFFFAOYSA-N

Formula:

C16H30O4Si3

SMILES:

C[Si](C)(C)OC(=O)c1cc(O[Si](C)(C)C)ccc1O[Si](C)(C)C

Mol. weight [g/mol]:

370.66

CAS:

3618-20-0

Physical Properties

Property code	Value	Unit	Source
log10ws	1.38		Crippen Method
logp	5.106		Crippen Method
rinpol	1800.00		NIST Webbook
rinpol	1801.00		NIST Webbook
rinpol	1801.00		NIST Webbook
rinpol	1802.00		NIST Webbook
rinpol	1802.00		NIST Webbook
rinpol	1802.00		NIST Webbook
rinpol	1803.00		NIST Webbook
rinpol	1777.00		NIST Webbook
rinpol	1777.00		NIST Webbook
rinpol	1794.00		NIST Webbook
rinpol	1801.00		NIST Webbook
rinpol	1798.00		NIST Webbook
rinpol	1798.00		NIST Webbook
rinpol	1796.00		NIST Webbook
rinpol	1779.00		NIST Webbook
rinpol	1783.00		NIST Webbook
rinpol	1782.00		NIST Webbook
rinpol	1764.40		NIST Webbook

rmpol	1780.00	NIST Webbook
rmpol	1783.00	NIST Webbook
rmpol	1793.00	NIST Webbook
rmpol	1797.00	NIST Webbook
rmpol	1783.00	NIST Webbook
rmpol	1791.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3618200&Units=SI

Legend

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

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