

Benzoic acid, 3,4,5-tris(trimethylsiloxy)-, trimethylsilyl ester

Other names:

Gallic acid, tetraTMS

Gallic acid, TMS

Benzoic acid, 3,4,5-tris-trimethylsilyloxy, trimethylsilyl ester

Gallic acid, 4tms derivative

Inchi:

InChI=1S/C19H38O5Si4/c1-25(2,3)21-16-13-15(19(20)24-28(10,11)12)14-17(22-26(4,5))

InchiKey:

KCIFUQKNKZTHGI-UHFFFAOYSA-N

Formula:

C19H38O5Si4

SMILES:

C[Si](C)(C)OC(=O)c1cc(O[Si](C)(C)C)c(O[Si](C)(C)C)c(O[Si](C)(C)C)c1

Mol. weight [g/mol]:

458.84

CAS:

2078-17-3

Physical Properties

Property code	Value	Unit	Source
log10ws	2.37		Crippen Method
logp	6.319		Crippen Method
rinpol	1990.00		NIST Webbook
rinpol	1991.00		NIST Webbook
rinpol	1991.00		NIST Webbook
rinpol	1991.00		NIST Webbook
rinpol	1994.00		NIST Webbook
rinpol	1994.00		NIST Webbook
rinpol	1995.00		NIST Webbook
rinpol	1962.00		NIST Webbook
rinpol	1962.00		NIST Webbook
rinpol	1984.00		NIST Webbook
rinpol	1991.00		NIST Webbook
rinpol	1987.00		NIST Webbook
rinpol	1986.00		NIST Webbook
rinpol	1983.00		NIST Webbook
rinpol	1976.00		NIST Webbook
rinpol	1978.60		NIST Webbook
rinpol	1983.00		NIST Webbook
rinpol	1981.00		NIST Webbook
rinpol	1987.00		NIST Webbook
rinpol	1994.00		NIST Webbook
rinpol	1984.00		NIST Webbook
rinpol	1976.00		NIST Webbook

rmpol	1983.00	NIST Webbook
rmpol	1978.60	NIST Webbook
rmpol	1978.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2078173&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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