

Benzoic acid trimethylsilyl ester

Other names:	Silanol, trimethyl-, benzoate Trimethylbenzoxysilane Trimethylsilyl benzoate Benzoyloxytrimethylsilane Monotrimethylsilyl derivative of benzoic acid Trimethylsilyl ester of benzoic acid Benzoic acid, monoTMS Benzoic acid, TMS Benzoic acid, TMS ester Benzoic acid, tms derivative
Inchi:	InChI=1S/C10H14O2Si/c1-13(2,3)12-10(11)9-7-5-4-6-8-9/h4-8H,1-3H3
InchiKey:	VFFKJJOXNCSJSAQ-UHFFFAOYSA-N
Formula:	C10H14O2Si
SMILES:	<chem>C[Si](C)(C)OC(=O)c1ccccc1</chem>
Mol. weight [g/mol]:	194.30
CAS:	2078-12-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.60		Crippen Method
logp	2.678		Crippen Method
rinpol	1232.00		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1226.00		NIST Webbook
rinpol	1248.00		NIST Webbook
rinpol	1230.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1229.00		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1267.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1242.00		NIST Webbook
rinpol	1248.00		NIST Webbook
rinpol	1249.00		NIST Webbook

rmpol	1250.00	NIST Webbook
rmpol	1248.00	NIST Webbook
rmpol	1257.00	NIST Webbook
rmpol	1226.00	NIST Webbook
rmpol	1233.00	NIST Webbook
rmpol	1267.00	NIST Webbook

Sources

Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2078128&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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