

Benzoic acid, 2-methoxy-, trimethylsilyl ester

Other names:	Trimethylsilyl 2-methoxybenzoate O-anisic acid, tms derivative
Inchi:	InChI=1S/C11H16O3Si/c1-13-10-8-6-5-7-9(10)11(12)14-15(2,3)4/h5-8H,1-4H3
InchiKey:	LWBFIZBQVRDUMY-UHFFFAOYSA-N
Formula:	C11H16O3Si
SMILES:	COc1ccccc1C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	224.33
CAS:	25436-32-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.72		Crippen Method
logp	2.687		Crippen Method
rinpol	1469.00		NIST Webbook
rinpol	1431.00		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=C25436322&Units=SI

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/22-460-6/Benzoic-acid-2-methoxy-trimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-04-26 18:05:55.173342499 +0000 UTC m=+16444004.093919815.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.