

Trimethylsilyl acetylsalicylate

Other names:	Benzoic acid, 2-(acetyloxy)-, trimethylsilyl ester Salicylic acid, trimethylsilyl ester, acetate Trimethylsilyl ester of acetylsalicylic acid Trimethylsilyl 2-(acetyloxy)benzoate Benzoic acid, 2-acetoxy, TMS Aspirin, tms derivative
Inchi:	InChI=1S/C12H16O4Si/c1-9(13)15-11-8-6-5-7-10(11)12(14)16-17(2,3)4/h5-8H,1-4H3
InchiKey:	GTMQKSKQHOCIDW-UHFFFAOYSA-N
Formula:	C12H16O4Si
SMILES:	<chem>CC(=O)Oc1ccccc1C(=O)O[Si](C)(C)C</chem>
Mol. weight [g/mol]:	252.34
CAS:	25436-28-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.92		Crippen Method
logp	2.604		Crippen Method
rinpol	1872.00		NIST Webbook
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Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25436286&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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