

3-Aminosalicylic acid, ethoxycarbonylated, TBDMS

Inchi:	InChI=1S/C22H39NO5Si2/c1-12-26-20(25)23-17-15-13-14-16(18(17)27-29(8,9)21(2,3)4)
InchiKey:	QQPMBULQPJLFFO-UHFFFAOYSA-N
Formula:	C22H39NO5Si2
SMILES:	CCOC(=O)Nc1cccc(C(=O)O[Si](C)(C)C(C)(C)C)c1O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	453.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.81		Crippen Method
logp	6.801		Crippen Method
rinpol	2528.00		NIST Webbook
rinpol	2528.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R563369&Units=SI

Legend

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

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<https://www.chemeo.com/cid/124-058-0/3-Aminosalicylic-acid-ethoxycarbonylated-TBDMS.pdf>

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