

4-Aminosalicylic acid, ethoxycarbonylated, TBDMS

Inchi:	InChI=1S/C22H39NO5Si2/c1-12-26-20(25)23-16-13-14-17(19(24)28-30(10,11)22(5,6)7)1
InchiKey:	VZFUYJQFSUHESD-UHFFFAOYSA-N
Formula:	C22H39NO5Si2
SMILES:	CCOC(=O)Nc1ccc(C(=O)O[Si](C)(C)C(C)(C)C)c(O[Si](C)(C)C(C)(C)C)c1
Mol. weight [g/mol]:	453.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.81		Crippen Method
logp	6.801		Crippen Method
rinpol	2673.00		NIST Webbook
rinpol	2673.00		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=R563656&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/113-302-0/4-Aminosalicylic-acid-ethoxycarbonylated-TBDMS.pdf>

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