

5-Aminosalicylic acid, ethoxycarbonylated, TBDMS

Inchi:	InChI=1S/C21H37NO5Si2/c1-20(2,3)28(8,9)26-17-13-12-15(22-19(24)25-7)14-16(17)18(
InchiKey:	QIMYTV AHLXGCQI-UHFFFAOYSA-N
Formula:	C21H37NO5Si2
SMILES:	COC(=O)Nc1ccc(O[Si](C)(C)C(C)(C)C)c(C(=O)O[Si](C)(C)C(C)(C)C)c1
Mol. weight [g/mol]:	439.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.39		Crippen Method
logp	6.411		Crippen Method
rinpol	2643.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R563829&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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