

1-O-trans-p-Coumaroylglycerol, 3TMS

Inchi:	InChI=1S/C21H38O5Si3/c1-27(2,3)24-17-20(26-29(7,8)9)16-23-21(22)15-12-18-10-13-1
InchiKey:	XIKYLENERWEDIW-NTCAYCPXSA-N
Formula:	C21H38O5Si3
SMILES:	C[Si](C)(C)OCC(COC(=O)C=Cc1ccc(O[Si](C)(C)C)cc1)O[Si](C)(C)C
Mol. weight [g/mol]:	454.78
CAS:	1048040-87-4

Physical Properties

Property code	Value	Unit	Source
log10ws	1.26		Crippen Method
logp	5.528		Crippen Method
rinpol	2494.60		NIST Webbook
rinpol	2494.60		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1048040874&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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.chemeo.com/cid/94-587-7/1-O-trans-p-Coumaroylglycerol-3TMS.pdf>

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