

Glyceryl ferulate, 3TMS

Inchi:	InChI=1S/C22H40O6Si3/c1-24-21-15-18(11-13-20(21)28-31(8,9)10)12-14-22(23)25-16-1
InchiKey:	CMGYIQVZEKYVKS-WYMLVPIESA-N
Formula:	C22H40O6Si3
SMILES:	COc1cc(C=CC(=O)OCC(CO[Si](C)(C)C)O[Si](C)(C)C)ccc1O[Si](C)(C)C
Mol. weight [g/mol]:	484.81
CAS:	307306-79-2

Physical Properties

Property code	Value	Unit	Source
log10ws	1.14		Crippen Method
logp	5.537		Crippen Method
rinsol	2629.40		NIST Webbook
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C307306792&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/95-830-5/Glyceryl-ferulate-3TMS.pdf>

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