

tert-Butyldimethylsilyl dodecyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, dodecyl tert-butyldimethylsilyl ester
Inchi:	InChI=1S/C26H44O4Si/c1-7-8-9-10-11-12-13-14-15-18-21-29-24(27)22-19-16-17-20-23(
InchiKey:	XXAGZSYBKRPALT-UHFFFAOYSA-N
Formula:	C26H44O4Si
SMILES:	CCCCCCCCCCCCOC(=O)c1cccc1C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	448.71

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.70		Crippen Method
logp	7.926		Crippen Method
rinpol	2852.00		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=U373697&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/66-031-4/tert-Butyldimethylsilyl-dodecyl-phthalate.pdf>

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