

Hexadecyl trimethylsilyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, hexadecyl trimethylsilyl ester
Inchi:	InChI=1S/C27H46O4Si/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-20-23-30-26(28)24-21-18
InchiKey:	FSSQLNRBQLPFW-UHFFFAOYSA-N
Formula:	C27H46O4Si
SMILES:	CCCCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	462.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.12		Crippen Method
logp	8.316		Crippen Method
rinpol	3113.00		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=U373706&Units=SI

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/44-555-7/Hexadecyl-trimethylsilyl-phthalate.pdf>

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