

3,5,5-Trimethylhexyl trimethylsilyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, 3,5,5-trimethylhexyl trimethylsilyl ester
Inchi:	InChI=1S/C20H32O4Si/c1-15(14-20(2,3)4)12-13-23-18(21)16-10-8-9-11-17(16)19(22)24
InchiKey:	NDUFIPOLFVTFAM-UHFFFAOYSA-N
Formula:	C20H32O4Si
SMILES:	CC(CCOC(=O)c1cccc1C(=O)O[Si](C)(C)C)CC(C)(C)C
Mol. weight [g/mol]:	364.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.71		Crippen Method
logp	5.297		Crippen Method
rinpol	2188.00		NIST Webbook
rinpol	2188.00		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=U373816&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/62-673-6/3-5-5-Trimethylhexyl-trimethylsilyl-phthalate.pdf>

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