

Trimethylsilyl undecyl phthalate

Other names: 1,2-Benzenedicarboxylic acid, undecyl trimethylsilylsilyl ester
Inchi: InChI=1S/C22H36O4Si/c1-5-6-7-8-9-10-11-12-15-18-25-21(23)19-16-13-14-17-20(19)22
InchiKey: ZVMNEIMGFNNOIK-UHFFFAOYSA-N
Formula: C22H36O4Si
SMILES: CCCCCCCCCCOC(=O)c1cccc1C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 392.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.03		Crippen Method
logp	6.366		Crippen Method
rinpol	2518.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U373702&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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/55-909-2/Trimethylsilyl-undecyl-phthalate.pdf>

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