

tert-Butyldimethylsilyl heptyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, heptyl tert-butyldimethylsilyl ester
Inchi:	InChI=1S/C21H34O4Si/c1-7-8-9-10-13-16-24-19(22)17-14-11-12-15-18(17)20(23)25-26(
InchiKey:	MQIOYOONYWNP HH-UHFFFAOYSA-N
Formula:	C ₂₁ H ₃₄ O ₄ Si
SMILES:	CCCCCCCOC(=O)c1cccc1C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	378.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.61		Crippen Method
logp	5.976		Crippen Method
rinpol	2348.00		NIST Webbook
rinpol	2348.00		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=U373647&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/53-161-4/tert-Butyldimethylsilyl-heptyl-phthalate.pdf>

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