

2-Ethylbutyl trimethylsilyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, 2-ethylbutyl trimethylsilyl ester
Inchi:	InChI=1S/C17H26O4Si/c1-6-13(7-2)12-20-16(18)14-10-8-9-11-15(14)17(19)21-22(3,4)5/
InchiKey:	FCLNZYRTQSWYGZ-UHFFFAOYSA-N
Formula:	C17H26O4Si
SMILES:	CCC(CC)COC(=O)c1ccccc1C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	322.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.70		Crippen Method
logp	4.271		Crippen Method
rinpol	1973.00		NIST Webbook
rinpol	1973.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373693&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/15-926-7/2-Ethylbutyl-trimethylsilyl-phthalate.pdf>

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