

1,3-Dioxoisobenzofuran-5-carboxylic acid, trimethylsilyl ester

Other names:	Trimethylsilyl 1,3-dioxoisobenzofuran-5-carboxylate Trimethylsilyl 1,3-dioxo-1,3-dihydro-2-benzofuran-5-carboxylate
Inchi:	InChI=1S/C12H12O5Si/c1-18(2,3)17-10(13)7-4-5-8-9(6-7)12(15)16-11(8)14/h4-6H,1-3H3
InchiKey:	IRIWFZRDYLPYBE-UHFFFAOYSA-N
Formula:	C12H12O5Si
SMILES:	C[Si](C)(C)OC(=O)c1ccc2c(c1)C(=O)OC2=O
Mol. weight [g/mol]:	264.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.06		Crippen Method
logp	1.989		Crippen Method
rinpol	1803.00		NIST Webbook
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373325&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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