

Trimethylsilyl 5-nitrofuran-2-carboxylate

Other names:	5-Nitrofuran-2-carboxylic acid, trimethylsilyl ester
Inchi:	InChI=1S/C8H11NO5Si/c1-15(2,3)14-8(10)6-4-5-7(13-6)9(11)12/h4-5H,1-3H3
InchiKey:	LTONXTDFGYBAOX-UHFFFAOYSA-N
Formula:	C8H11NO5Si
SMILES:	<chem>C[Si](C)(C)OC(=O)c1ccc([N+](=O)[O-])o1</chem>
Mol. weight [g/mol]:	229.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.99		Crippen Method
logp	2.179		Crippen Method
rinpol	1477.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378222&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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/61-847-4/Trimethylsilyl-5-nitrofuran-2-carboxylate.pdf>

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