2-Furoic acid, 2,2,2-trichloroethyl ester

Inchi:	InChI=1S/C7H5Cl3O3/c8-7(9,10)4-13-6(11)5-2-1-3-12-5/h1-3H,4H2
InchiKey:	WWHZWLUAKBBFNX-UHFFFAOYSA-N
Formula:	C7H5Cl3O3
SMILES:	O=C(OCC(Cl)(Cl)Cl)c1ccco1
Mol. weight [g/mol]:	243.47
CAS:	63938-48-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.43		Crippen Method
logp	2.807		Crippen Method
mcvol	140.060	ml/mol	McGowan Method
rinpol	1473.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63938487&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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