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: 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
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.