

4-(2-[2-(2,4,6-Trichlorophenoxy)ethoxy]ethyl)morpholine

Inchi:	InChI=1S/C14H18Cl3NO3/c15-11-9-12(16)14(13(17)10-11)21-8-7-20-6-3-18-1-4-19-5-2-
InchiKey:	KWVTWZARCZTHEV-UHFFFAOYSA-N
Formula:	C14H18Cl3NO3
SMILES:	Clc1cc(Cl)c(OCCOCCN2CCOCC2)c(Cl)c1
Mol. weight [g/mol]:	354.66
CAS:	116401-63-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.22		Crippen Method
logp	3.374		Crippen Method
mcvol	237.810	ml/mol	McGowan Method

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=C116401639&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

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