N-[2,2,2-trichloro-1-[4-(2,2,2-trichloro-1-formamido

Inchi: InChI=1S/C10H14Cl6N4O2/c11-9(12,13)7(17-5-21)19-1-2-20(4-3-19)8(18-6-22)10(14,15

InchiKey: RROQIUMZODEXOR-UHFFFAOYSA-N

Formula: C10H14Cl6N4O2

SMILES: O=CNC(N1CCN(C(NC=O)C(Cl)(Cl)Cl)CC1)C(Cl)(Cl)Cl

Mol. weight [g/mol]: 434.97

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.19		Aqueous Solubility Prediction Method
logp	1.489		Crippen Method
mcvol	257.400	ml/mol	McGowan Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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