

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(CI)(CI)CI)CC1)C(CI)(CI)CI
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/AqueousDataset002.xlsx>

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

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.cheméo.com/cid/102-821-6/N-2-2-2-trichloro-1-4-2-2-2-trichloro-1-formamidoethyl-piperazin-1-yl-ethyl-formamide>

Generated by Cheméo on 2024-05-05 02:19:10.034139075 +0000 UTC m=+17164798.954716391.

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