Trichloroacetic acid, morpholide

Inchi: InChI=1S/C6H8Cl3NO2/c7-6(8,9)5(11)10-1-3-12-4-2-10/h1-4H2
InchiKey: GDPGGCADYVWIBK-UHFFFAOYSA-N
Formula: C6H8Cl3NO2
SMILES: O=C(N1CCOCC1)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 232.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.22		Crippen Method
logp	1.215		Crippen Method
mcvol	138.680	ml/mol	McGowan Method
rinpol	1470.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U307213&Units=SI
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

Legend

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