

4-Trichloroacetyl morpholine

Inchi:	InChI=1S/C6H8Cl3NO3/c7-6(8,9)13-5(11)10-1-3-12-4-2-10/h1-4H2
InchiKey:	JTGCUGQAAWWAIF-UHFFFAOYSA-N
Formula:	C6H8Cl3NO3
SMILES:	O=C(OC(Cl)(Cl)Cl)N1CCOCC1
Mol. weight [g/mol]:	248.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.78		Crippen Method
logp	1.783		Crippen Method
mcvol	144.550	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=B6002275&Units=SI
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

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<https://www.chemeo.com/cid/59-670-3/4-Trichloroacetyl-morpholine.pdf>

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