

Piperidine, 1-trichloroacetyl-

Inchi:	InChI=1S/C7H10Cl3NO/c8-7(9,10)6(12)11-4-2-1-3-5-11/h1-5H2
InchiKey:	COHUYGSEUCDFQT-UHFFFAOYSA-N
Formula:	C7H10Cl3NO
SMILES:	O=C(N1CCCCC1)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	230.52
CAS:	2296-53-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.55		Crippen Method
logp	2.369		Crippen Method
mcvol	146.900	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=C2296539&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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<https://www.chemeo.com/cid/21-020-5/Piperidine-1-trichloroacetyl.pdf>

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