

Glycouril, 1,3,4,6-tetrachloro-

Other names:	1,3,4,6-tetrachlorotetrahydroimidazo[4,5-d]imidazole-2,5(1H,3H)-dione
Inchi:	InChI=1S/C4H2Cl4N4O2/c5-9-1-2(11(7)3(9)13)12(8)4(14)10(1)6/h1-2H
InchiKey:	TWVLNKKMSLYUQQ-UHFFFAOYSA-N
Formula:	C4H2Cl4N4O2
SMILES:	O=C1N(Cl)C2C(N1Cl)N(Cl)C(=O)N2Cl
Mol. weight [g/mol]:	279.90
CAS:	776-19-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.86		Crippen Method
logp	1.729		Crippen Method
mcvol	137.520	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C776192&Units=SI

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.chemeo.com/cid/80-723-0/Glycouril-1-3-4-6-tetrachloro.pdf>

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