

Dichlorocyanuric acid

Other names:	dichloro-1,3,5-triazinetriene
Inchi:	InChI=1S/C3HCl2N3O3/c4-7-1(9)6-2(10)8(5)3(7)11/h(H,6,9,10)
InchiKey:	CEJLBZWIKQJOAT-UHFFFAOYSA-N
Formula:	C3HCl2N3O3
SMILES:	O=c1nc(O)n(Cl)c(=O)n1Cl
Mol. weight [g/mol]:	197.96
CAS:	2782-57-2

Physical Properties

Property code	Value	Unit	Source
log10ws	0.02		Crippen Method
logp	-0.886		Crippen Method
mcvol	101.400	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2782572&Units=SI
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

Legend

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

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