

1,2,3-Benzotriazine-4-(3h)-one, 6,8-dichloro-

Inchi:	InChI=1S/C7H3Cl2N3O/c8-3-1-4-6(5(9)2-3)10-12-11-7(4)13/h1-2H,(H,10,11,13)
InchiKey:	QZJXNGLZXVQFIJ-UHFFFAOYSA-N
Formula:	C7H3Cl2N3O
SMILES:	O=c1[nH]nnc2c(Cl)cc(Cl)cc12
Mol. weight [g/mol]:	216.02
CAS:	60233-65-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.82		Crippen Method
logp	1.143		Crippen Method
mcvol	126.560	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60233650&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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