

Purine, 2,6,8-trichloro-

Other names:	2,6,8-trichloropurine
Inchi:	InChI=1S/C5HCl3N4/c6-2-1-3(11-4(7)9-1)12-5(8)10-2/h(H,9,10,11,12)
InchiKey:	XPTCECRKQRKFLH-UHFFFAOYSA-N
Formula:	C5HCl3N4
SMILES:	Clc1nc(Cl)c2[nH]c(Cl)nc2n1
Mol. weight [g/mol]:	223.45
CAS:	2562-52-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.85		Crippen Method
logp	1.831		Crippen Method
mcvol	119.030	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2562529&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Latest version available from:

<https://www.chemeo.com/cid/72-963-3/Purine-2-6-8-trichloro.pdf>

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