

Melamine, hexachloro-

Inchi:	InChI=1S/C3Cl6N6/c4-13(5)1-10-2(14(6)7)12-3(11-1)15(8)9
InchiKey:	VCBRTBDPBXC BOR-UHFFFAOYSA-N
Formula:	C3Cl6N6
SMILES:	C1N(Cl)c1nc(N(Cl)Cl)nc(N(Cl)Cl)n1
Mol. weight [g/mol]:	332.79
CAS:	2428-04-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.84		Crippen Method
logp	3.214		Crippen Method
mcvol	162.690	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2428048&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

Latest version available from:

<https://www.chemeo.com/cid/75-903-6/Melamine-hexachloro.pdf>

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