

Benzimidazole, 4,5,6,7-tetrachloro-2-(trifluoromethyl)-

Inchi:	InChI=1S/C8HCl4F3N2/c9-1-2(10)4(12)6-5(3(1)11)16-7(17-6)8(13,14)15/h(H,16,17)
InchiKey:	QLKDMIUEWFNEPV-UHFFFAOYSA-N
Formula:	C8HCl4F3N2
SMILES:	FC(F)(F)c1nc2c(Cl)c(Cl)c(Cl)c(Cl)c2[nH]1
Mol. weight [g/mol]:	323.91
CAS:	2338-29-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.10		Crippen Method
logp	4.713		Crippen Method
mcvol	158.890	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2338296&Units=SI

Legend

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

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