

Benzimidazole, 4,5,6-trichloro-2-(trifluoromethyl)-

Inchi:	InChI=1S/C8H2Cl3F3N2/c9-2-1-3-6(5(11)4(2)10)16-7(15-3)8(12,13)14/h1H,(H,15,16)
InchiKey:	BXCSXZJKEJQDKS-UHFFFAOYSA-N
Formula:	C8H2Cl3F3N2
SMILES:	FC(F)(F)c1nc2c(Cl)c(Cl)c(Cl)cc2[nH]1
Mol. weight [g/mol]:	289.47
CAS:	2338-27-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.42		Crippen Method
logp	4.060		Crippen Method
mcvol	146.650	ml/mol	McGowan Method

Sources

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=C2338274&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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