

Benzimidazole, 4,6,7-trichloro-2-(trifluoromethyl)-

Inchi:	InChI=1S/C8H2Cl3F3N2/c9-2-1-3(10)5-6(4(2)11)16-7(15-5)8(12,13)14/h1H,(H,15,16)
InchiKey:	ZVFDYQZOXSAMSR-UHFFFAOYSA-N
Formula:	C8H2Cl3F3N2
SMILES:	FC(F)(F)c1nc2c(Cl)cc(Cl)c(Cl)c2[nH]1
Mol. weight [g/mol]:	289.47
CAS:	3393-59-7

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3393597&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

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<https://www.chemeo.com/cid/63-953-4/Benzimidazole-4-6-7-trichloro-2-trifluoromethyl.pdf>

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