

1H-Benzimidazole, 5,6-dichloro-2-(trifluoromethyl)-

Other names:	Benzimidazole, 5,6-dichloro-2-(trifluoromethyl)- NC 2983 5,6-Dichloro-2-Trifluoromethylbenzimidazole
Inchi:	InChI=1S/C8H3Cl2F3N2/c9-3-1-5-6(2-4(3)10)15-7(14-5)8(11,12)13/h1-2H,(H,14,15)
InchiKey:	KUMRUFFLHYXFLV-UHFFFAOYSA-N
Formula:	C8H3Cl2F3N2
SMILES:	FC(F)(F)c1nc2cc(Cl)c(Cl)cc2[nH]1
Mol. weight [g/mol]:	255.02
CAS:	2338-25-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.73		Crippen Method
logp	3.407		Crippen Method
mcvol	134.410	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=C2338252&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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