

Benzimidazole, 4,6-dichloro-5-nitro-2-(trifluoromethyl)-

Inchi:	InChI=1S/C8H2Cl2F3N3O2/c9-2-1-3-5(4(10)6(2)16(17)18)15-7(14-3)8(11,12)13/h1H,(H,
InchiKey:	ABRYUUSJZZOGOI-UHFFFAOYSA-N
Formula:	C8H2Cl2F3N3O2
SMILES:	O=[N+]([O-])c1c(Cl)cc2[nH]c(C(F)(F)F)nc2c1Cl
Mol. weight [g/mol]:	300.02
CAS:	6609-43-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.39		Crippen Method
logp	3.315		Crippen Method
mcvol	151.830	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=C6609434&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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