

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

Inchi:	InChI=1S/C8H2Cl2F3N3O2/c9-4-3(16(17)18)1-2-6(5(4)10)15-7(14-2)8(11,12)13/h1H,(H,
InchiKey:	TZMZZAAWGRCWAY-UHFFFAOYSA-N
Formula:	C8H2Cl2F3N3O2
SMILES:	O=[N+]([O-])c1cc2[nH]c(C(F)(F)F)nc2c(Cl)c1Cl
Mol. weight [g/mol]:	300.02
CAS:	6609-42-3

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6609423&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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