

# Benzimidazole, 4-chloro-6-nitro-2-(trifluoromethyl)-

Inchi:	InChI=1S/C8H3ClF3N3O2/c9-4-1-3(15(16)17)2-5-6(4)14-7(13-5)8(10,11)12/h1-2H,(H,13)
InchiKey:	HNDQGIJHWSTKDW-UHFFFAOYSA-N
Formula:	C8H3ClF3N3O2
SMILES:	O=[N+]([O-])c1cc(Cl)c2nc(C(F)(F)F)[nH]c2c1
Mol. weight [g/mol]:	265.58
CAS:	4228-91-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.70		Crippen Method
logp	2.661		Crippen Method
mcvol	139.590	ml/mol	McGowan Method

## Sources

NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4228915&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4228915&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

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

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