# 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:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C4228915&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**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