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

Inchi: InChI=1S/C8H3ClF3N3O2/c9-3-1-4-6(5(2-3)15(16)17)14-7(13-4)8(10,11)12/h1-2H,(H,13

InchiKey: STOJWTVNHAJLBI-UHFFFAOYSA-N

Formula: C8H3ClF3N3O2

SMILES: O=[N+]([O-])c1cc(Cl)cc2[nH]c(C(F)(F)F)nc12

Mol. weight [g/mol]: 265.58

CAS: 3671-18-9

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3671189&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

Latest version available from:

https://www.chemeo.com/cid/45-078-6/Benzimidazole-6-chloro-4-nitro-2-trifluoromethyl.pdf

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