Benzimidazole, 4,6-dinitro-2-(trifluoromethyl)-

Inchi: InChI=1S/C8H3F3N4O4/c9-8(10,11)7-12-4-1-3(14(16)17)2-5(15(18)19)6(4)13-7/h1-2H,(H

InchiKey: ABJSFSLMGRVNBG-UHFFFAOYSA-N

Formula: C8H3F3N4O4

SMILES: O=[N+]([O-])c1cc([N+](=O)[O-])c2nc(C(F)(F)F)[nH]c2c1

Mol. weight [g/mol]: 276.13

CAS: 6609-38-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.67		Crippen Method
logp	1.916		Crippen Method
mcvol	144.770	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=C6609387&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