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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6609387&Units=SI

Legend

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

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