Nicotinonitrile, 2-hydroxy-6-methyl-5-nitro-4-(trifluoromethyl)-, (keto form)

Inchi: InChI=1S/C8H4F3N3O3/c1-3-6(14(16)17)5(8(9,10)11)4(2-12)7(15)13-3/h1H3,(H,13,15)
InchiKey: VBZATTIMIASLRS-UHFFFAOYSA-N
Formula: C8H4F3N3O3
SMILES: Cc1[nH]c(=O)c(C#N)c(C(F)(F)F)c1[N+](=O)[O-]
Mol. weight [g/mol]: 247.13
CAS: 651-77-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.70		Crippen Method
logp	1.000		Crippen Method
mcvol	139.780	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=C651774&Units=SI

Legend

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