

Nicotinonitrile, 2-chloro-6-methyl-5-nitro-4-(trifluoromethyl)-

Inchi:	InChI=1S/C8H3ClF3N3O2/c1-3-6(15(16)17)5(8(10,11)12)4(2-13)7(9)14-3/h1H3
InchiKey:	FNSVJEGHKFDQGK-UHFFFAOYSA-N
Formula:	C8H3ClF3N3O2
SMILES:	Cc1nc(Cl)c(C#N)c(C(F)(F)F)c1[N+](=O)[O-]
Mol. weight [g/mol]:	265.58
CAS:	783-95-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.51		Crippen Method
logp	2.842		Crippen Method
mcvol	146.150	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C783959&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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