Benzimidazole, 5-nitro-2-(trifluoromethyl)-

Inchi: InChI=1S/C8H4F3N3O2/c9-8(10,11)7-12-5-2-1-4(14(15)16)3-6(5)13-7/h1-3H,(H,12,13)
InchiKey: FEJRBJIEEALTTL-UHFFFAOYSA-N
Formula: C8H4F3N3O2
SMILES: O=[N+]([O-])c1ccc2[nH]c(C(F)(F)F)nc2c1
Mol. weight [g/mol]: 231.13
CAS: 327-19-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.02		Crippen Method
logp	2.008		Crippen Method
mcvol	127.350	ml/mol	McGowan Method

Sources

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=C327195&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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