1-Methyl-2-trifluoro-methyl benzimidazole

Inchi: InChI=1S/C9H7F3N2/c1-14-7-5-3-2-4-6(7)13-8(14)9(10,11)12/h2-5H,1H3
InchiKey: YKKYRNSRLGCTDO-UHFFFAOYSA-N
Formula: C9H7F3N2
SMILES: Cn1c(C(F)(F)F)nc2ccccc21
Mol. weight [g/mol]: 200.16
CAS: 384-46-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.43		Crippen Method
logp	2.592		Crippen Method
mcvol	124.020	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=C384463&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