1-(2-Trifluoromethylphenyl)imidazole

Inchi: InChI=1S/C10H7F3N2/c11-10(12,13)8-3-1-2-4-9(8)15-6-5-14-7-15/h1-7H
InchiKey: WZBWBNCQUTXYEL-UHFFFAOYSA-N
Formula: C10H7F3N2
SMILES: FC(F)(F)c1ccccc1-n1ccnc1
Mol. weight [g/mol]: 212.17
CAS: 25371-96-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.99		Crippen Method
logp	2.891		Crippen Method
mcvol	133.810	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C25371964&Units=SI
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

Legend

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