1-(4-Trifluoromethylphenyl)imidazole

Inchi: InChI=1S/C10H7F3N2/c11-10(12,13)8-1-3-9(4-2-8)15-6-5-14-7-15/h1-7H
InchiKey: FUJKJTAYTFLIDA-UHFFFAOYSA-N
Formula: C10H7F3N2
SMILES: FC(F)(F)c1ccc(-n2ccnc2)cc1
Mol. weight [g/mol]: 212.17
CAS: 25371-98-6

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

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=C25371986&Units=SI

Legend

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

Latest version available from:
https://www.chemeo.com/cid/122-905-1/1-4-Trifluoromethylphenyl-imidazole.pdf
Generated by Cheméo on 2024-04-28 09:35:21.207820656 +0000 UTC m=+16586170.128397968.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.