

1-(3-Trifluoromethylphenyl)imidazole

Other names:	Imidazole, 1-(3-trifluoromethylphenyl)-
Inchi:	InChI=1S/C10H7F3N2/c11-10(12,13)8-2-1-3-9(6-8)15-5-4-14-7-15/h1-7H
InchiKey:	KZVUPVJLOACZIL-UHFFFAOYSA-N
Formula:	C10H7F3N2
SMILES:	FC(F)(F)c1cccc(-n2ccnc2)c1
Mol. weight [g/mol]:	212.17
CAS:	25371-97-5

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25371975&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.chemeo.com/cid/69-289-6/1-3-Trifluoromethylphenyl-imidazole.pdf>

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