

5-Benzimidazole carbonitrile, 2-(trifluoromethyl)-

Inchi:	InChI=1S/C9H4F3N3/c10-9(11,12)8-14-6-2-1-5(4-13)3-7(6)15-8/h1-3H,(H,14,15)
InchiKey:	PMISAFNVEGVLSS-UHFFFAOYSA-N
Formula:	C9H4F3N3
SMILES:	N#Cc1ccc2[nH]c(C(F)(F)F)nc2c1
Mol. weight [g/mol]:	211.14
CAS:	3671-61-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.72		Crippen Method
logp	1.971		Crippen Method
mcvol	125.400	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=C3671612&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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