2-Trifluoromethylbenzimidazole

Other names:	Benzimidazole, 2-(trifluoromethyl)-
Inchi:	InChI=1S/C8H5F3N2/c9-8(10,11)7-12-5-3-1-2-4-6(5)13-7/h1-4H,(H,12,13)
InchiKey:	MXFMPTXDHSDMTI-UHFFFAOYSA-N
Formula:	C8H5F3N2
SMILES:	FC(F)(F)c1nc2ccccc2[nH]1
Mol. weight [g/mol]:	186.13
CAS:	312-73-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.36		Crippen Method
logp	2.100		Crippen Method
mcvol	109.930	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=C312732&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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