

2-Trifluoromethyl-5-methoxybenzimidazole

Other names:	Benzimidazole, 5-methoxy-2-(trifluoromethyl)-
Inchi:	InChI=1S/C9H7F3N2O/c1-15-5-2-3-6-7(4-5)14-8(13-6)9(10,11)12/h2-4H,1H3,(H,13,14)
InchiKey:	GPYQJBAVCKSQJTJ-UHFFFAOYSA-N
Formula:	C9H7F3N2O
SMILES:	COc1ccc2[nH]c(C(F)(F)F)nc2c1
Mol. weight [g/mol]:	216.16
CAS:	3671-65-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.48		Crippen Method
logp	2.108		Crippen Method
mcvol	129.890	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=C3671656&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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