

Benzimidazole, 2,5-bis(trifluoromethyl)-

Inchi:	InChI=1S/C9H4F6N2/c10-8(11,12)4-1-2-5-6(3-4)17-7(16-5)9(13,14)15/h1-3H,(H,16,17)
InchiKey:	BKFXAUQYNCJXIZ-UHFFFAOYSA-N
Formula:	C9H4F6N2
SMILES:	FC(F)(F)c1ccc2[nH]c(C(F)(F)F)nc2c1
Mol. weight [g/mol]:	254.13
CAS:	399-69-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.47		Crippen Method
logp	3.119		Crippen Method
mcvol	129.330	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C399699&Units=SI
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

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/67-999-0/Benzimidazole-2-5-bis-trifluoromethyl.pdf>

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