

Benzimidazole, 4,5,7-trifluoro-

Inchi:	InChI=1S/C7H3F3N2/c8-3-1-4(9)6-7(5(3)10)12-2-11-6/h1-2H,(H,11,12)
InchiKey:	LKGYJXCGRGDDIA-UHFFFAOYSA-N
Formula:	C7H3F3N2
SMILES:	Fc1cc(F)c2[nH]cnc2c1F
Mol. weight [g/mol]:	172.11
CAS:	2686-72-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.26		Crippen Method
logp	1.498		Crippen Method
mcvol	95.840	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C2686728&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/36-047-0/Benzimidazole-4-5-7-trifluoro.pdf>

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