

Benzimidazole, 4,7-dibromo-2-(trifluoromethyl)-

Inchi:	InChI=1S/C8H3Br2F3N2/c9-3-1-2-4(10)6-5(3)14-7(15-6)8(11,12)13/h1-2H,(H,14,15)
InchiKey:	DYLVHVMRWJVLNS-UHFFFAOYSA-N
Formula:	C8H3Br2F3N2
SMILES:	FC(F)(F)c1nc2c(Br)ccc(Br)c2[nH]1
Mol. weight [g/mol]:	343.93
CAS:	4228-97-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.69		Crippen Method
logp	3.625		Crippen Method
mcvol	144.930	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4228971&Units=SI
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

Legend

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

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