

Benzimidazole, 4,6-dibromo-2-(trifluoromethyl)-

Inchi:	InChI=1S/C8H3Br2F3N2/c9-3-1-4(10)6-5(2-3)14-7(15-6)8(11,12)13/h1-2H,(H,14,15)
InchiKey:	IPVBKOUKUCKNIK-UHFFFAOYSA-N
Formula:	C8H3Br2F3N2
SMILES:	FC(F)(F)c1nc2c(Br)cc(Br)cc2[nH]1
Mol. weight [g/mol]:	343.93
CAS:	6609-53-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.69		Crippen Method
logp	3.625		Crippen Method
mvol	144.930	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=C6609536&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.chemeo.com/cid/35-103-8/Benzimidazole-4-6-dibromo-2-trifluoromethyl.pdf>

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