

Benzimidazole, 4-bromo-2-(trifluoromethyl)-

Inchi:	InChI=1S/C8H4BrF3N2/c9-4-2-1-3-5-6(4)14-7(13-5)8(10,11)12/h1-3H,(H,13,14)
InchiKey:	MWSWJWXZVTVPEQ-UHFFFAOYSA-N
Formula:	C8H4BrF3N2
SMILES:	FC(F)(F)c1nc2c(Br)cccc2[nH]1
Mol. weight [g/mol]:	265.03
CAS:	6587-23-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.53		Crippen Method
logp	2.862		Crippen Method
mcvol	127.430	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=C6587231&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

Latest version available from:

<https://www.chemeo.com/cid/50-260-7/Benzimidazole-4-bromo-2-trifluoromethyl.pdf>

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