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: 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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6587231&Units=SI

Legend

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