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: DYLHVMDRWJVLSN-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/ci990307l
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