



Formula: C3H6BrNO4

MW: 199.99

CAS: 52-51-2

MDL NUMBER: MFCD00007390

IUPAC: 2-bromo-2-nitropropane-1,3-diol

Smiles: C(CO)(CO)(Br)[N+](O)=O

THERAPEUTIC CATEGORY: ANTISEPTIC

ACCEPTORS: 4

DONORS: 2

ROTATION BONDS: 4

N+O: 5

Chiral Centers: 0

LogP: -0.9

LogS: -2.06

LIPINSKI: 4

