

Bis(5-nitroimidazole-4-carboxamido)ethylene

Inchi: InChI=1S/C10H10N8O6/c19-9(5-7(17(21)22)15-3-13-5)11-1-2-12-10(20)6-8(18(23)24)16
InchiKey: AYZXXRUQQTXZDM-UHFFFAOYSA-N
Formula: C10H10N8O6
SMILES: O=C(NCCNC(=O)c1nc[nH]c1[N+](=O)[O-])c1nc[nH]c1[N+](=O)[O-]
Mol. weight [g/mol]: 338.24

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.08 | | Crippen Method |
| logp | -1.855 | | Crippen Method |
| mcvol | 210.700 | 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=B6008325&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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