s-2,3-DIAMINOPROPYL DIHYDROGEN PHOSPHOROTHIOATE

Other names: S-2,3-Diaminopropyl dihydrogen phosphorothioate
Propylthiophosphonic acid, 2,3-diamino-
Inchi: InChI=1S/C3H11N2O3PS/c4-1-3(5)2-10-9(6,7)8/h3H,1-2,4-5H2,(H2,6,7,8)
InchiKey: TXLJMOJYKYDULH-UHFFFAOYSA-N
Formula: C3H11N2O3PS
SMILES: NCC(N)CSP(=O)(O)O
Mol. weight [g/mol]: 186.17

Physical Properties

Property code	Value	Unit	Source
logp	-0.902		Crippen Method
mcvol	127.510	ml/mol	McGowan Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C78219008&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume