Phosphorothioic acid, S-2,3-diaminopropyl ester

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
CAS: 78219-00-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.73		Crippen Method
logp	-0.902		Crippen Method
mcvol	127.510	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=C78219008&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.