

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

Latest version available from:

<https://www.chemeo.com/cid/81-247-8/s-2-3-DIAMINOPROPYL-DIHYDROGEN-PHOSPHOROTHIOATE.pdf>

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