

# S-Ethyl S-(2-diisopropylaminoethyl) methylphosphonodithioate

Other names:

S-Ethyl-S-[2-(diisopropylamino)ethyl]methylphosphonothiodithiolate

S-Ethyl S-[2-(diisopropylamino)ethyl]methylphosphonothiolate

Methyldithiophosphonic acid, S-ethyl, S-(2-diisopropylaminoethyl) ester

Inchi:

InChI=1S/C11H26NOPS2/c1-7-15-14(6,13)16-9-8-12(10(2)3)11(4)5/h10-11H,7-9H2,1-6H

InchiKey:

WALRJEDABGCYFW-UHFFFAOYSA-N

Formula:

C11H26NOPS2

SMILES:

CCSP(C)(=O)SCCN(C(C)C)C(C)C

Mol. weight [g/mol]:

283.43

CAS:

110501-55-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.26		Crippen Method
logp	4.414		Crippen Method
mcvol	234.860	ml/mol	McGowan Method
rinpol	1760.00		NIST Webbook
rinpol	1793.10		NIST Webbook
rinpol	1760.00		NIST Webbook
rinpol	1793.10		NIST Webbook
rinpol	1760.00		NIST Webbook
rinpol	1760.00		NIST Webbook

## Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C110501558&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](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  
**rinpol:** Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/31-418-3/S-Ethyl-S-2-diisopropylaminoethyl-methylphosphonodithioate.pdf>

Generated by Cheméo on 2024-04-30 00:48:09.178441988 +0000 UTC m=+16727338.099019303.

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