S-Isobutyl, S-2-(diethylamino)ethyl methyldithiophosphonate

Inchi: InChI=1S/C12H28NOPS2/c1-6-13(7-2)9-8-10-16-15(5,14)17-11-12(3)4/h12H,6-11H2,1-5

InchiKey: HOXQFIUTXXEYJH-UHFFFAOYSA-N

Formula: C12H28NOPS2

SMILES: CCN(CC)CCCSP(C)(=O)SCC(C)C

Mol. weight [g/mol]: 297.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.22		Crippen Method
logp	4.664		Crippen Method
mcvol	248.950	ml/mol	McGowan Method
rinpol	1782.00		NIST Webbook
rinpol	1782.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R403777&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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