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

Inchi: InChI=1S/C13H30NOPS3/c1-6-14(7-2)8-9-17-10-11-18-16(5,15)19-12-13(3)4/h13H,6-12
InchiKey: RWJDEYBNSGEHBZ-UHFFFAOYSA-N
Formula: C13H30NOPS3
SMILES: CCN(CC)CCSCCSP(C)(=O)SCC(C)C
Mol. weight [g/mol]: 343.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.52		Crippen Method
logp	5.007		Crippen Method
mcvol	279.390	ml/mol	McGowan Method
rinpol	2128.00		NIST Webbook
rinpol	2128.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R403762&Units=SI

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.