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

Inchi: InChI=1S/C14H32NOPS4/c1-6-15(7-2)13-19-9-8-18-10-11-20-17(5,16)21-12-14(3)4/h14H
InchiKey: GDFWDHPWQQVCTF-UHFFFAOYSA-N
Formula: C14H32NOPS4
SMILES: CCN(CC)CSCCSCCSP(C)(=O)SCC(C)C
Mol. weight [g/mol]: 389.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.32		Crippen Method
logp	5.697		Crippen Method
mcvol	309.830	ml/mol	McGowan Method
rinpol	2636.00		NIST Webbook
rinpol	2636.00		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=R403757&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.