o,o'-Dipropyl allyl phosphonothioate

Inchi: InChI=1S/C9H19O2PS/c1-4-7-10-12(13,9-6-3)11-8-5-2/h6H,3-5,7-9H2,1-2H3
InchiKey: IGDFSGPDLZOZPR-UHFFFAOYSA-N
Formula: C9H19O2PS
SMILES: C=CCP(=S)(OCCC)OCCC
Mol. weight [g/mol]: 222.28
CAS: 77659-29-1

Physical Properties

Property code	Value	Unit	Source
ie	8.50	eV	NIST Webbook
ie	8.86	eV	NIST Webbook
log10ws	1.12		Crippen Method
logp	3.335		Crippen Method
mcvol	181.920	ml/mol	McGowan Method

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=C77659291&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume