Isothioate

Inchi: InChI=1S/C7H17O2PS3/c1-7(2)12-5-6-13-10(11,8-3)9-4/h7H,5-6H2,1-4H3
InchiKey: SPCNPOWOBZQWJK-UHFFFAOYSA-N
Formula: C7H17O2PS3
SMILES: COP(=S)(OC)SCCSC(C)C
Mol. weight [g/mol]: 260.38
CAS: 36614-38-7

Physical Properties

Property code	Value	Unit	Source
log10ws	0.94		Crippen Method
logp	3.379		Crippen Method
mcvol	190.740	ml/mol	McGowan Method
rinpol	1720.00		NIST Webbook
rinpol	1720.00		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=C36614387&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