

Propyl phosphorotrithioite

Inchi:	InChI=1S/C9H21PS3/c1-4-7-11-10(12-8-5-2)13-9-6-3/h4-9H2,1-3H3
InchiKey:	ADRLBSFJQOGKCV-UHFFFAOYSA-N
Formula:	C9H21PS3
SMILES:	CCCSP(SCCC)SCCC
Mol. weight [g/mol]:	256.43
CAS:	869-56-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.07		Crippen Method
logp	5.643		Crippen Method
mcvol	207.180	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C869567&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/57-695-8/Propyl-phosphorotrithioite.pdf>

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