

Phosphorotrithious acid, trimethyl ester

Inchi: InChI=1S/C3H9PS3/c1-5-4(6-2)7-3/h1-3H3
InchiKey: FVTIMWPYAZCZQB-UHFFFAOYSA-N
Formula: C3H9PS3
SMILES: CSP(SC)SC
Mol. weight [g/mol]: 172.27
CAS: 816-80-8

Physical Properties

Property code	Value	Unit	Source
ie	7.70	eV	NIST Webbook
ie	8.42	eV	NIST Webbook
log10ws	0.44		Crippen Method
logp	3.302		Crippen Method
mcvol	122.640	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C816808&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie: Ionization energy
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/109-979-5/Phosphorotrithious-acid-trimethyl-ester.pdf>

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