

Tributyl phosphorotrithioite

Other names:	Merphos Phosphorotrithious acid, tributyl ester Butyl phosphorotrithioite ((BuS)3P) Tributyl trithiophosphite Chemagro B-1776 Deleaf defoliant Easy off-D Folex Phosphorotrithious acid, S,S,S-tributyl ester S,S,S-Tributyl phosphorotrithioite S,S,S-Tributyl trithiophosphite Tributylthiofosfin NSC 27720 Tris(butylthio)phosphine S,S',S'-tributyl phosphorotrithioite
Inchi:	InChI=1S/C12H27PS3/c1-4-7-10-14-13(15-11-8-5-2)16-12-9-6-3/h4-12H2,1-3H3
InchiKey:	KLAPGAOQRZTCBI-UHFFFAOYSA-N
Formula:	C12H27PS3
SMILES:	CCCCSP(SCCCC)SCCCC
Mol. weight [g/mol]:	298.51
CAS:	150-50-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.32		Crippen Method
logp	6.813		Crippen Method
mcvol	249.450	ml/mol	McGowan Method

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=C150505&Units=SI

Legend

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

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