

S,S,S-Tributyl phosphorotrithioate

Other names:	B-1,776 Butifos Butiphos Butyl Phosphorotrithioate ((BuS)3PO) Butyl phosphorotrithioate Chemagro 1,776 Chemagro B-1776 DEF DEF Defoliant De-Green E-Z-Off D Fos-Fall A Fosfall Merphos oxide Merphos-oxon Merphos-oxone Ortho phosphate defoliant Phosphorotrithioic acid, S,S,S-tributyl ester S,S,S-Tributyl trithiophosphate S,S,S-Tributyltrithiofosfat TBTP Tribufos Tribuphos Tributyl phosphorotrithioate
Inchi:	InChI=1S/C12H27OPS3/c1-4-7-10-15-14(13,16-11-8-5-2)17-12-9-6-3/h4-12H2,1-3H3
InchiKey:	ZOKXUAHZSKEQSS-UHFFFAOYSA-N
Formula:	C12H27OPS3
SMILES:	CCCCSP(=O)(SCCCC)SCCCC
Mol. weight [g/mol]:	314.51
CAS:	78-48-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.14		Aqueous Solubility Prediction Method
log10ws	-5.14		Estimated Solubility Method

logp	6.694		Crippen Method
mcvol	255.320	ml/mol	McGowan Method
ripol	2771.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C78488&Units=SI>

Legend

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

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