

Phosphorotrithioic acid, S,S,S-tributyl ester

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
	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]:	314.52

Physical Properties

Property code	Value	Unit	Source
hf	-386.48	kJ/mol	Cheméo Relay (1.0)
hvap	84.09	kJ/mol	Cheméo Relay (1.0)
ie	8.45	eV	Cheméo Relay (1.0)
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
rinpol	2142.00		NIST Webbook
rinpol	2188.00		NIST Webbook
rinpol	2193.00		NIST Webbook
rinpol	2117.00		NIST Webbook
ripol	2771.00		NIST Webbook
ripol	2771.00		NIST Webbook
tb	618.23	K	Cheméo Relay (1.0)
tf	234.59	K	Cheméo Relay (1.0)

Sources

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

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

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

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

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/75-342-9/Phosphorotriethioic-acid-S-S-S-tributyl-ester.pdf>

Generated by Cheméo on 2026-07-24 09:43:50.843342407 +0000 UTC m=+397326.685227788.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.