Phosphorotrithious acid, tributyl ester

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]:	298.52

Physical Properties

Property code	Value	Unit	Source
hf	-179.88	kJ/mol	Cheméo Relay (1.0)
hvap	77.03	kJ/mol	Cheméo Relay (1.0)
ie	7.43	eV	Cheméo Relay (1.0)
logp	6.813		Crippen Method
mcvol	249.450	ml/mol	McGowan Method
tb	610.31	K	Cheméo Relay (1.0)
tf	243.71	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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C150505&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point