Phosphonothioic acid, phenyl-, O-ethyl O-(4-nitrophenyl) ester

Other names: Phosphonothioic acid, phenyl-, O-ethyl O-(p-nitrophenyl) ester
EPN 300
O-Ethyl O-(p-nitrophenyl) benzenethiophosphonate
O-Ethyl O-(p-nitrophenyl) phenylphosphonothioate
O-Ethyl O-(4-nitrophenyl) benzenethionophosphonate
O-Ethyl O-(4-nitrophenyl) phenylphosphonothioate
Benzenephosphonic acid, thiono-, ethyl-(p-nitrophenyl) ester
Ethoxy-(((4-nitrophenoxy)phenyl)phosphine) sulfide
Ethyl (p-nitrophenyl) benzenethionophosphonate
Ethyl (p-nitrophenyl) benzenethiophosphate
Ethyl (p-nitrophenyl) benzenethiophosphonate
Ethyl (p-nitrophenyl) phenylphosphonothioate
Ethyl (p-nitrophenyl) thionobenzenephosphate
Ethyl (p-nitrophenyl) thionobenzenephosphonate
ENT 17,798
O-Aethyl-O-(4-nitro-phenyl)-phenyl-monothiophosphonat
O-Ethyl phenyl (p-nitrophenyl) thiophosphonate
O-Ethyl O-(p-nitrophenyl) phenylphosphonothiolate
O-Ethyl O-(p-nitrophenyl) phenylphosphorothioate
O-Ethyl-O-((4-nitro-fenyl)-fenyl)-monothiofosfonaat
O-Etil-O-((4-ntiro-fenil)-fenil)-monotiofosfonato
Phenol, p-nitro-, O-ester with O-ethyl phenyl phosphonothioate
Phenylphosphonothioate, O-ethyl-O-p-nitrophenyl-
Phenylthiophosphonate de O-ethyle et O-4-nitrophenyle
PIN
Santox
O-Ethyl-O-p-nitrofenylester kyseliny fenylthiofosfonove
O-(4-Nitrophenyl) O-ethyl phenyl thiophosphonate
OMS 219
Phenylphosphonothioic acid O-ethyl O-p-nitrophenyl ester
EPN
NSC 404840
NSC 8943

Inchi: InChI=1S/C14H14NO4PS/c1-2-18-20(21,14-6-4-3-5-7-14)19-13-10-8-12(9-11-13)15(16)1

InchiKey: AIGRXSNSLVJMEA-UHFFFAOYSA-N

Formula: C14H14NO4PS

SMILES: CCOP(=S)(Oc1ccc([N+](=O)[O-])cc1)c1ccccc1

Mol. weight [g/mol]: 323.30

CAS: 2104-64-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.01		Crippen Method
logp	3.645		Crippen Method
mcvol	226.570	ml/mol	McGowan Method
rinpol	2460.00		NIST Webbook
rinpol	2460.00		NIST Webbook
rinpol	2460.00		NIST Webbook
tf	309.59 ± 0.20	K	NIST Webbook
tf	312.00 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	25.05	kJ/mol	308.20	NIST Webbook
hfust	25.05	kJ/mol	308.20	NIST Webbook
hfust	25.05	kJ/mol	308.20	NIST Webbook

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=C2104645&Units=SI

Legend

hfust: Enthalpy of fusion at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

tf: Normal melting (fusion) point