Phoxim

Other names:

(Diethoxy-thiophosphoryloxyimino)-phenyl acetonitrile
2-(Diethoxyphosphinothioyloxyimino)-2-phenylacetonitrile
3,5-Dioxa-6-aza-4-phosphaoct-6-ene-8-nitrile, 4-ethoxy-7-phenyl-, 4-sulfide
4-Ethoxy-7-phenyl-3,5-dioxa-6-aza-4-phosphaoct-6-ene-8-nitril 4-sulfide
4-Ethoxy-7-phenyl-3,5-dioxa-6-aza-4-phosphaoct-6-ene-8-nitrile 4-sulfide
B 77488
BAY 5621
BAY 77488
BAY SRA 7502
Bayer 5621
Bayer 77488
Bayer 9053
Baythion
Benzeneacetonitrile, [[(diethoxyphosphinothioyl)oxy]imino]-
Benzeneacetonitrile, «alpha»-[[(diethoxyphosphinothioyl)oxy]imino]-
Benzeneacetonitrile, Â«alphaÂ»-[[(diethoxyphosphinothioyl)oxy]imino]-
Benzoyl cyanide O-(diethoxyphosphinothioyl)oxime
ENT 27488
Foxim
Foxima
Glyoxylonitrile, phenyl-, oxime O,O-diethyl phosphorothioate
N-Diethoxyphosphinothioyloxybenzimidoyl cyanide
O,O-Diaethyl-O-(«alpha»-cyanbenzyliden-amino)-thionphosphat
O,O-Diaethyl-O-(«alpha»-cyano-benzylidenamino)-monothiophosphat
O,O-Diaethyl-O-(Â«alphaÂ»-cyanbenzyliden-amino)-thionphosphat
O,O-Diaethyl-O-(Â«alphaÂ»-cyano-benzylidenamino)-monothiophosphat
O,O-Diethyl O-(«alpha»-cyanobenzylideneamino)phosphorothioate
O,O-Diethyl O-(Â«alphaÂ»-cyanobenzylideneamino)phosphorothioate
O,O-Diethyl phosphorothioate, O-ester with phenylglyoxylonitrile oxime
O,O-Diethyl «alpha»-cyanobenzylideneamino-oxyphosphonothioate
O,O-Diethyl Â«alphaÂ»-cyanobenzylideneamino-oxyphosphonothioate
O,O-Diethyl-«alpha»-cyanobenzylidineaminooxyphosphonothiate
O,O-Diethyl-Â«alphaÂ»-cyanobenzylidineaminooxyphosphonothiate
OMS 1170
Phenylglyoxylnitrile oxime O,O-diethyl phosphorothioate
Phenylglyoxylonitrile Oxime O,O-diethyl phosphorothioate
Phoxime
Phoxin
Sebacil
Valexon

	Valexone
	Volaton
	«alpha»-(((Diethoxyphosphinothioyl)oxy)imino)benzeneacetonitrile
	Â«alphaÂ»-(((Diethoxyphosphinothioyl)oxy)imino)benzeneacetonitrile
Inchi:	InChI=1S/C12H15N2O3PS/c1-3-15-18(19,16-4-2)17-14-12(10-13)11-8-6-5-7-9-11/h5-9H
InchiKey:	ATROHALUCMTWTB-UHFFFAOYSA-N
Formula:	C12H15N2O3PS
SMILES:	CCOP(=S)(OCC)ON=C(C#N)c1ccccc1
Mol. weight [g/mol]:	298.30
CAS:	14816-18-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.86		Aqueous Solubility Prediction Method
log10ws	-4.86		Estimated Solubility Method
logp	3.228		Crippen Method
mcvol	217.660	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14816183&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

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