O-(P-CYANOPHENYL) O-ETHYL PHENYLPHOSPHONOTHIOATE

Other names: Phosphonothioic acid, phenyl-, O-(4-cyanophenyl) O-ethyl ester
Phosphonothioic acid, phenyl-, O-ethyl ester, O-ester with p-hydroxybenzonitrile
B 10094
Cyanofenphos
CP 19699
CYP
Monsanto CP-19699
O-Ethyl O-(4-cyanophenyl) phenylphosphonothioate
OMS 870
S 4087
Surazon
Surecide
Benzonitrile, p-hydroxy-, O-ester with O-ethyl phenylphosphonothioate
O-p-Cyanophenyl O-ethyl phenyl-phosphonothioate
O-(4-Cyanophenyl) O-ethyl phenylphosphonothioate
ENT 25,832
ENT 25,832-a
O-Ethyl phenylphosphonothioate, O-ester with p-hydroxybenzonitrile
Experimental insecticide S-4087
Phenylphosphonothioic acid O-ethyl ester O-ester with p-hydroxybenzonitrile
Stauffer B-10094
Upjohn U-32714

Inchi: InChI=1S/C15H14NO2PS/c1-2-17-19(20,15-6-4-3-5-7-15)18-14-10-8-13(12-16)9-11-14/h

InchiKey: LRNJHZNPJSPMGK-UHFFFAOYSA-N

Formula: C15H14NO2PS

SMILES: CCOP(=S)(Oc1ccc(C#N)cc1)c1ccccc1

Mol. weight [g/mol]: 303.32

Physical Properties

Property code	Value	Unit	Source
ie	8.42	eV	Cheméo Relay (1.0)
logp	3.609		Crippen Method
mcvol	224.620	ml/mol	McGowan Method
rinpol	2245.00		NIST Webbook
rinpol	2236.00		NIST Webbook
rinpol	2260.00		NIST Webbook

rinpol	2245.00		NIST Webbook
rinpol	2243.00		NIST Webbook
rinpol	2252.00		NIST Webbook
rinpol	2260.00		NIST Webbook
rinpol	2243.00		NIST Webbook
rinpol	2268.00		NIST Webbook
rinpol	2252.00		NIST Webbook
rinpol	2268.00		NIST Webbook
tb	667.60	K	Cheméo Relay (1.0)
tf	311.38	K	Cheméo Relay (1.0)

Sources

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=C13067931&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point