

Cyanophos

Other names:	Phosphorothioic acid, O-(4-cyanophenyl) O,O-dimethyl ester O-4-Cyanophenyl O,O-dimethyl phosphorothioate Phosphorothioic acid, O,O-dimethyl ester, O-ester with p-hydroxybenzotrile BAY 34727 BAYER 34727 Ciafos O-p-Cyanophenyl O,O-dimethyl phosphorothioate Cyanox CYAP O,O-Dimethyl-O-(4-cyano-phenyl)-monothiophosphate O,O-Dimethyl-O-p-cyanophenyl phosphorothioate O,O-Dimethyl O-4-cyanophenyl phosphorothioate O,O-Dimethyl O-4-cyanophenyl thiophosphate ENT 25,675 MAY & BAKER S-4084 OMS 226 OMS 869 S 4084 Sumitomo S 4084
Inchi:	InChI=1S/C9H10NO3PS/c1-11-14(15,12-2)13-9-5-3-8(7-10)4-6-9/h3-6H,1-2H3
InchiKey:	SCKHCCSZFPSHGR-UHFFFAOYSA-N
Formula:	C9H10NO3PS
SMILES:	COP(=S)(OC)Oc1ccc(C#N)cc1
Mol. weight [g/mol]:	243.22
CAS:	2636-26-2

Physical Properties

Property code	Value	Unit	Source
log10ws	1.21		Crippen Method
logp	2.454		Crippen Method
mcpol	169.710	ml/mol	McGowan Method
rinpol	1700.00		NIST Webbook
rinpol	1776.00		NIST Webbook
rinpol	1733.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1735.00		NIST Webbook
rinpol	1781.00		NIST Webbook

rinpol	1776.00	NIST Webbook
rinpol	1704.00	NIST Webbook
rinpol	1730.00	NIST Webbook
ripol	2866.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C2636262&Units=SI

Legend

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

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