

Phosphorothioic acid, S-[2-[(1-cyano-1-methylethyl)amino]-2-oxoethyl] O,O-diethyl ester

Other names:

Phosphorothioic acid, O,O-diethyl ester, S-ester with N-(1-cyano-1-methylethyl)-2-mercaptoacetamide
Cyanthoate

M 1568

Tartan

Phosphorothioic acid, S-(((1-cyano-1-methyl-ethyl)carbamoyl)methyl) O,O-diethyl ester
«alpha»-Cyanoisopropylamide of O,O-diethylthiophosphoryl acetic acid

S-(((1-Cyano-1-methyl-ethyl)carbamoyl)methyl) O,O-diethyl phosphorothioate

S-N-(1-Cyano-1-methylethyl)carbamoylmethyl diethyl phosphorothiolate

O,O-Diethyl-S-((2-cyaan-2-methyl-ethyl)-carbamoyl)-methyl-monothiofosfaat

O,O-Diethyl-S-N-(«alpha»-cyanoisopropyl)carbomoylmethyl phosphorothioate

O,O-Dietil-S-((2-cian-2-metil-etil)-carbamoil)-metil-monotiofosfato

TH-427-1

Thiophosphate de S-N-(1-cyano-1-methylethyl)carbamoylmethyle et de O,O-diethyle

Inchi: InChI=1S/C10H19N2O4PS/c1-5-15-17(14,16-6-2)18-7-9(13)12-10(3,4)8-11/h5-7H2,1-4H

InchiKey: TWDJIKFUVRYBJF-UHFFFAOYSA-N

Formula: C10H19N2O4PS

SMILES: CCOP(=O)(OCC)SCC(=O)NC(C)(C)C#N

Mol. weight [g/mol]: 294.31

CAS: 3734-95-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.27		Crippen Method
logp	2.319		Crippen Method
mvol	219.110	ml/mol	McGowan Method

Sources

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=C3734950&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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