Pyrazophos

Other names:	Pyrazolo[1,5-a]pyrimidine-6-carboxylic acid, 2-[(diethoxyphosphinothioyl)oxy]-5-methyl-, ethyl ester Pyrazolo[1,5-a]pyrimidine-6-carboxylic acid, 2-hydroxy-5-methyl-, ethyl ester, O-ester with O,O-diethyl phosphorothioate Afugan Hoechst 2873 HOE 2873 Curamil Ethyl 2-hydroxy-5-methylpyrazolo(1,5-a)pyrimidine-6-carboxylate O-ester of O,O-diethylphosphorothioic acid Ethyl 2-((diethoxyphosphinothioyl)oxy)-5-methylpyrazolo(1,5-a)pyrimidine-6-carboxylate Pyrazolo(1,5a)pyrimidine, 2-(O,O-diethyl thionophosphoryl)-5-methyl-6-ethoxycarbonyl- 2-(O,O-Diethyl thionophosphoryl)-5-methyl-6-carbethoxy-pyrazolo(1,5a)pyrimidin Phosphorothioic acid, O,O-diethyl ester, O-ester with (6-ethoxycarbonyl-5-methyl)pyrazolo(1,5-a)pyrimidin-2-ol O,O-Diethyl-O-(5-methyl-6-ethoxy-carbonyl-pyrazolo(1.5-a)pyrimid-2-yl)-thionophosphate 2-(O,O-Diethyl-thionophosphoryl)-5-methyl-6-carbethoxy-pyrazolo-(1,5-a)pyrimidine Missile NSC 232671 O-6-ethoxycarbonyl-5-methylpyrazolo[1,5-a]pyrimidin-2-yl O,O-diethyl phosphorothioate
Inchi:	InChI=1S/C14H20N3O5PS/c1-5-19-14(18)11-9-17-12(15-10(11)4)8-13(16-17)22-23(24,2
InchiKey:	JOOMJVFZQRQWKR-UHFFFAOYSA-N
Formula:	C14H20N3O5PS
SMILES:	CCOC(=O)c1cn2nc(OP(=S)(OCC)OCC)cc2nc1C
Mol. weight [g/mol]:	373.36
CAS:	13457-18-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.90		Crippen Method
logp	2.891		Crippen Method
mcvol	261.000	ml/mol	McGowan Method
rinpol	2622.00		NIST Webbook
tf	325.23 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

hfust	27.32	kJ/mol	324.40	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13457186&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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