

Dialifor

Other names:

2-(2-chloro-1-diethoxyphosphinothioylsulfanylethyl)isoindole-1,3-dione

Dialifos

Dialiphor

Dialiphos

ENT 27320

Hercules 14503

O,O-Diaethyl-S-2-chlor-1-(phthalimido)-aethyl-dithiophosphat

O,O-Diethyl S-(2-chloro-1-phthalimidoethyl)phosphorodithioate

Phosphorodithioic acid, O,O-diethyl ester, S-ester with

N-(2-chloro-1-mercaptoethyl)phthalimide

Phosphorodithioic acid, S-(2-chloro-1-phthalimidoethyl) O,O-diethyl ester

Phosphorodithioic acid,

S-[2-chloro-1-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)ethyl] O,O-diethyl ester

S-(2-Chloro-1-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)ethyl) O,O-diethyl

phosphorodithioate

S-(2-Chloro-1-phthalimidoethyl) O,O-diethyl phosphorodithioate

Torak

Inchi: InChI=1S/C14H17ClNO4PS2/c1-3-19-21(22,20-4-2)23-12(9-15)16-13(17)10-7-5-6-8-11(18)**InchiKey:** MUMQYXACQUZOFU-UHFFFAOYSA-N**Formula:** C14H17ClNO4PS2**SMILES:** CCOP(=S)(OCC)SC(CCl)N1C(=O)c2ccccc2C1=O**Mol. weight [g/mol]:** 393.85**CAS:** 10311-84-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.03		Aqueous Solubility Prediction Method
log10ws	-6.34		Estimated Solubility Method
logp	3.878		Crippen Method
mcvol	263.760	ml/mol	McGowan Method
rinpol	2553.00		NIST Webbook
tf	341.23 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10311849&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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