Phosphorothioic acid, O-(3-chloro-4-nitrophenyl) O,O-dimethyl ester

Other names:	BAY 22190
	Bayer 22/190
	Chloorthion
	Chlorothion
	Chlorthion Methyl
	Chlortion
	Compound 22/190
	Dimethyl 3-chloro-4-nitrophenyl thionophosphate
	ENT 18,861
	Methyl chlorothion
	NSC 8927
	O,O-Dimethyl O-(3-chloro-4-nitrophenyl) phosphorothioate
	O,O-Dimethyl O-(3-chloro-4-nitrophenyl) thiophosphate
	O,O-Dimethyl O-4-nitro-3-chlorophenyl thiophosphate
	O,O-Dimethyl p-nitro-m-chlorophenyl thiophosphate
	O,O-Dimethyl-O-(3-chlor-4-nitrophenyl)-monothiophosphat
	O,O-Dimethyl-O-(4-nitro-5-chlorphenyl)-thionophosphat
	O,O-Dimethyl-O-3-chlor-4-nitrofenylester kyseliny thiofosforecne
	O,O-Dimethyl-O-3-chlor-4-nitrofenyltiofosfat
	O-(3-Chloor-4-nitro-fenyl)-O,O-dimethyl-monothiofosfaat
	O-(3-Chlor-4-nitro-phenyl)-O,O-dimethyl-monothiophosphat
	O-(3-Chloro-4-nitro-fenyl)-O,O-dimethyl-monothiofosfaat
	O-(3-Chloro-4-nitrophenyl) O,O-dimethyl phosphorothioate
	O-(3-Cloro-4-nitro-fenil)-O,O-dimetil-monotiofosfato
	O-(3-chloro-4-nitrophenyl) O,O-dimethyl thiophosphate
	OMS 217
	Phenol, 3-chloro-4-nitro-, O-ester with O,O-dimethyl phosphorothioate
	Thiophosphate de O,O-dimethyle et de O-3-chloro-4-nitrophenyle
	p-Nitro-m-chlorophenyl dimethyl thionophosphate
Inchi:	InChI=1S/C8H9ClNO5PS/c1-13-16(17,14-2)15-6-3-4-8(10(11)12)7(9)5-6/h3-5H,1-2H3
InchiKey:	NZNRRXXETLSZRO-UHFFFAOYSA-N
Formula:	C8H9ClNO5PS
SMILES:	COP(=S)(OC)Oc1ccc([N+](=O)[O-])c(Cl)c1
Mol. weight [g/mol]:	297.66
CAS:	500-28-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.63		Cheméo Relay (1.0)
logp	3.144		Crippen Method
mcvol	183.900	ml/mol	McGowan Method
rinpol	1945.00		NIST Webbook
rinpol	1964.00		NIST Webbook
rinpol	1991.00		NIST Webbook
tb	609.69	K	Cheméo Relay (1.0)
tf	289.64	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	92.00	kJ/mol	346.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.35129e+01
Coeff. B	-1.10704e+04
Temperature range (K), min.	476.65
Temperature range (K), max.	608.22

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C500287&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
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):

Legend

hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point