o-(2-Chloro-4-nitrophenyl) o,o-dimethyl phosphorothioate

Other names: AC 4124
American Cyanamid 4124
American cyanamid 4,124
BAY 14981
BAYER 22/190
Captec
Dicaptan
Dicapthion
Dicapthon
Dicapton
Dimethyl 2-chloronitrophenyl thiophosphate
ENT 17,035
Experimental Insecticide 4124
Insecticide ACC 4124
Isochloorthion
Isochlorothion
Isochlorthion
Isomeric Chlorthion
O,O-Dimethyl O-2-chloro-4-nitrophenyl phosphorothioate
O,O-Dimethyl-O-(2-chloro-4-nitrophenyl)thionophosphate
O-(4-Chloor-3-nitro-fenyl)-O,O-dimethylmonothiofosfaat
O-(4-Chlor-3-nitro-phenyl)-O,O-dimethyl-monothiophosphat
O-(4-Cloro-3-nitro-fenil)-O,O-dimetil-monotiofosfato
OMS-214
Phenol, 2-chloro-4-nitro-, O-ester with O,O-dimethyl phosphorothioate
Phosphorothioic acid, O-(2-chloro-4-nitrophenyl) O,O-dimethyl ester
Thiophosphate de O,O-dimethyle et de O-4-chloro-3-nitrophenyle
dicaphton
p-Nitro-o-chlorophenyl dimethyl thionophosphate

Inchi: InChI=1S/C8H9ClNO5PS/c1-13-16(17,14-2)15-8-4-3-6(10(11)12)5-7(8)9/h3-5H,1-2H3

InchiKey: OTKXWJHPGBRXCR-UHFFFAOYSA-N

Formula: C8H9ClNO5PS

SMILES: COP(=S)(OC)Oc1ccc([N+](=O)[O-])cc1Cl

Mol. weight [g/mol]: 297.66

Physical Properties

Property code	Value	Unit	Source

hvap	86.09	kJ/mol	Cheméo Relay (1.0)
ie	9.20	eV	Cheméo Relay (1.0)
log10ws	-4.31		Aqueous Solubility Prediction Method
log10ws	-4.31		Estimated Solubility Method
logp	3.144		Crippen Method
mcvol	183.900	ml/mol	McGowan Method
tb	601.68	K	Cheméo Relay (1.0)
tf	325.65	K	Aqueous Solubility Prediction Method
tf	323.00 ± 0.20	K	NIST Webbook
tf	323.90 ± 0.10	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	29.08	kJ/mol	323.90	NIST Webbook
hfust	29.08	kJ/mol	323.90	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2463845&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hfust: Enthalpy of fusion at a given temperature

hvap: Enthalpy of vaporization at standard conditions

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point