

Dicaphthon

Other names:	AC 4124 American Cyanamid 4124 American cyanamid 4,124 BAY 14981 BAYER 22/190 Captac Dicaptan Dicaphthon Dicapton Dimethyl 2-chloronitrophenyl thiophosphate ENT 17,035 Experimental Insecticide 4124 Insecticide ACC 4124 Isochlorothion Isochlorothion Isochlorthion Isomeric Chlorthion O,O-Dimethyl O-2-chloro-4-nitrophenyl phosphorothioate O,O-Dimethyl-O-(2-chloro-4-nitrophenyl)thionophosphate O-(2-Chloro-4-nitrophenyl) O,O-dimethyl phosphorothioate O-(4-Chlor-3-nitro-fenyl)-O,O-dimethylmonothiofosfaat O-(4-Chlor-3-nitro-phenyl)-O,O-dimethyl-monothiophosphat O-(4-Chloro-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 dicaphthon 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:	<chem>COP(=S)(OC)Oc1ccc([N+](=O)[O-])cc1Cl</chem>
Mol. weight [g/mol]:	297.65
CAS:	2463-84-5

Physical Properties

Property code	Value	Unit	Source
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
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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2463845&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tf:	Normal melting (fusion) point

Latest version available from:

<https://www.cheméo.com/cid/15-415-4/Dicapthon.pdf>

Generated by Cheméo on 2024-04-20 06:18:35.737327129 +0000 UTC m=+15883164.657904445.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.