Phosalone

Other names:	11974 RP 3-[O,O-(Diethyldithiophosphoryl)methyl]-6-chlorobenzoxazolinone 6-Chloro-3-[O,O-(diethyldithiophosphoryl)methyl]benzoxazolone 6-chloro-3-(diethoxyphosphinothioylsulfanylmethyl)-1,3-benzoxazol-2-one Agria 1060 Azofene Benzophosphate Chipman 11974 ENT 27163 Fosalon Fosalone Fozalon NIA 9241 O,O-Diethyl phosphorodithioate S-ester with 6-chloro-3-(mercaptomethyl)-2-benzoxazolinone P 974 Phasolon Phosalon Phosphorodithioic acid, O,O-diethyl ester, S-ester with 6-chloro-3-(mercaptomethyl)-2-benzoxazolinone Phosphorodithioic acid, S-[(6-chloro-2-oxo-3(2H)-benzoxazolyl)methyl] O,O-diethyl ester Phozalon RP 11974 Rhodia RP 11974 Rubitox S-(6-Chloro-2-oxobenzoxazolin-3-yl)methyl diethyl phosphorothiolothionate S-6-chloro-2,3-dihydro-2-oxobenzoxazol-3-ylmethyl O,O-diethylphosphorodithioate S-[(6-Chloro-2-oxo-3(2H)-benzoxazoly)methyl] O,O-diethyl phosphorodithioate Zolone Zolone PM Zoolon
Inchi:	InChI=1S/C12H15ClNO4PS2/c1-3-16-19(20,17-4-2)21-8-14-10-6-5-9(13)7-11(10)18-12(1
InchiKey:	IOUNQDKNJZEDEP-UHFFFAOYSA-N
Formula:	C12H15ClNO4S2
SMILES:	CCOP(=S)(OCC)SCn1c(=O)oc2cc(Cl)ccc21
Mol. weight [g/mol]:	336.83
CAS:	2310-17-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.23		Aqueous Solubility Prediction Method
log10ws	-5.23		Estimated Solubility Method
logp	4.236		Crippen Method
mcvol	239.880	ml/mol	McGowan Method
rinpol	2488.00		NIST Webbook
rinpol	2461.00		NIST Webbook
rinpol	2476.00		NIST Webbook
rinpol	2537.00		NIST Webbook
rinpol	2480.00		NIST Webbook
rinpol	2537.00		NIST Webbook
rinpol	2480.00		NIST Webbook
rinpol	2537.00		NIST Webbook
rinpol	2476.00		NIST Webbook
tf	320.90	K	Aqueous Solubility Prediction Method
tf	321.56 ± 0.20	K	NIST Webbook
tf	321.90 ± 0.10	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	30.03	kJ/mol	320.00	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2310170&Units=SI

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

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