Bromophos

Other names:	(4-bromo-2,5-dichlorophenoxy)-dimethoxy-sulfanylidenephosphorane
	4-Bromo-2,5-Dichlorophenyl dimethyl phosphorothionate
	Brofene
	Bromofos
	Bromofos-Methyl
	Bromophos-methyl
	Bromovur
	Brophene
	Cela S 1942
	Cx99
	Drillzid
	EL 400
	ENT 27,162
	Metabrom
	Mexion
	NSC 527602
	Netal
	Nexagan
	Nexion
	Nexion 40
	Nexion 5G
	Nexion LC 40
	O,O-Dimethyl O-(2,5-dichloro-4-bromophenyl) phosphorothioate
	O,O-Dimethyl O-(2,5-dichloro-4-bromophenyl) thiophosphate
	O,O-Dimethyl O-(4-bromo-2,5-dichlorophenyl) phosphorothioate
	O-(4-Brom-2,5-dichlor-phenyl)-O,O-dimethyl-monothiophosphat
	O-(4-Bromo-2,5-dichlorophenyl) O,O-dimethyl phosphorothioate
	O-(4-Broom-2,5-dichloor-fenyl)-O,O-dimethyl-monothiofosfaat
	OMS 658
	Omexan
	Phenol, 4-bromo-2,5-dichloro-, O-ester with O,O-dimethyl phosphorothioate
	Phosphorothioic acid, O-(4-bromo-2,5-dichlorophenyl) O,O-dimethyl ester
	S 1942
	Sovinexion
	Thiophosphate de O,O-dimethyle et de O-4-bromo-2,5-dichlorophenyle
Inchi:	InChI=1S/C8H8BrCl2O3PS/c1-12-15(16,13-2)14-8-4-6(10)5(9)3-7(8)11/h3-4H,1-2H3
InchiKey:	NYQDCVLCJXRDSK-UHFFFAOYSA-N
Formula:	C8H8BrCl2O3PS
SMILES:	COP(=S)(OC)Oc1cc(Cl)c(Br)cc1Cl
Mol. weight [g/mol]:	366.00

CAS: 2104-96-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.09		Estimated Solubility Method
log10ws	-6.09		Aqueous Solubility Prediction Method
logp	4.652		Crippen Method
mcvol	196.220	ml/mol	McGowan Method
rinpol	1982.00		NIST Webbook
rinpol	1982.00		NIST Webbook
rinpol	2026.00		NIST Webbook
rinpol	1982.00		NIST Webbook
rinpol	2003.00		NIST Webbook
rinpol	2026.00		NIST Webbook
tf	329.00 ± 0.20	K	NIST Webbook
tf	325.89 ± 0.20	K	NIST Webbook
tf	326.65	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	31.15	kJ/mol	325.30	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2104963&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point