

Naled

Other names:	(1,2-dibromo-2,2-dichloroethyl) dimethyl phosphate 1,2-Dibromo-2,2-Dichloroethyl dimethyl phosphate 1,2-Dibromo-2,2-dichloroethyl dimethyl phosphatic acid Alvora BRP Bromchlophos Bromex Bromex (insecticide) Bromex 50 Dibrom Dibromfos Dimethyl 1,2-dibromo-2,2-dichloroethyl phosphate ENT 24988 Ethanol, 1,2-dibromo-2,2-dichloro-, dimethyl phosphate Flibol Ex Fosbrom O-(1,2-Dibromo-2,2-dichloroethyl)-O,O-dimethyl phosphate O-Dibrom 8E Ortho-Dibrom Phosphoric acid, 1,2-dibromo-2,2-dichloroethyl dimethyl ester RE 4355
Inchi:	InChI=1S/C4H7Br2Cl2O4P/c1-10-13(9,11-2)12-3(5)4(6,7)8/h3H,1-2H3
InchiKey:	BUYMVQAILCEWRR-UHFFFAOYSA-N
Formula:	C4H7Br2Cl2O4P
SMILES:	COP(=O)(OC)OC(Br)C(Cl)(Cl)Br
Mol. weight [g/mol]:	380.78
CAS:	300-76-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.28		Estimated Solubility Method
log10ws	-2.28		Aqueous Solubility Prediction Method
logp	3.651		Crippen Method
mcvol	170.640	ml/mol	McGowan Method
rinpol	1668.00		NIST Webbook

rinpol	1590.00	NIST Webbook
rinpol	1645.00	NIST Webbook
rinpol	1635.00	NIST Webbook
rinpol	1602.00	NIST Webbook
rinpol	1635.00	NIST Webbook
rinpol	1630.00	NIST Webbook
rinpol	1602.00	NIST Webbook
ripol	1930.00	NIST Webbook
ripol	1930.00	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C300765&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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