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Review

Partition coefficients (*n*-octanol–water) for pesticides

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ABSTRACT

Data for the partition coefficients (*n*-octanol–water) (P_{ow}) of 221 pesticides and pesticide metabolites are presented with their method of derivation and source. The methods of measurement and calculating log P_{ow} are reviewed. Octanol–water partition coefficients are measured by shake-flask methods, reversed-phase HPLC, reversed-phase TLC, slow-stirring partition methods and column generator method. Octanol–water partition coefficients are calculated from substituent constants, molecular fragment summation and solubilities. It has been proposed that the HPLC operating conditions for any compound should be applicable to other compounds which have the same log P_{ow}. The log P_{ow} may be used in estimating the environmental behaviour of pesticides. A classification of pesticides as fat-soluble has been proposed for compounds with a log $P_{ow} > 4$.

CONTENTS

1. INTRODUCTION

The partition coefficient (P) is defined as the ratio of the equilibrium concentrations of a dissolved substance in a two-phase system consisting of two largely immiscible solvents [1], in this case *n*-octanol and water. Octanol represents a substitute for biotic lipid and hence gives an approximation to a biotic lipid–water partition coefficient [2]. The ratio is reported as a logarithm usually as log P_{ow} or log K_{ow}.

Comprehensive data on partition coefficients have been published [3–5] however these cover a wide range of organic compounds and searching is required to find any pesticide of interest. The partition coefficients for some pesticides are given with other parameters in a published list of environmental data [6]. Because of the importance of the environmental effects of pesticides a detailed list of important parameters such as partition coefficients is necessary.

A number of techniques have been used to mea-

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sure or calculate log P_{ow}. Because of the range of methods used there is a wide discrepancy in the values reported [7]. To make decisions on the usefulness of these values it is necessary to have access to as many as possible and also to know their derivation.

The purpose of this review is to set out a comprehensive list of pesticides with their partition coefficients and the methods of derivation. Information on some metabolites is also included. Some uses of partition coefficients are also examined.

2. DIFFERENT METHODS OF MEASURING OR CALCULATING LOG P_{ow}

2.1. Experimental measurement

The classic measurement for log P_{ow} is the shake-flask method [1] where a compound is shaken in *n*-octanol–water and after equilibrium the concentration is measured in one or both phases. It can measure a range of log P_{ow} from -2.5 to 4.5, is applicable to most classes of compounds but is affected by impurities and difficult for compounds of low solubility [8]. Variations of the shake flask method include inversion [9–16], stirring [17], dissolved in octanol and water added before shaking [18] and shaking in a separating funnel [19].

Octanol–water partition coefficients have applications in many areas. Much research involves the development of new methods, to measure log P_{ow}, which are easier, more accurate, more reproducible and less time consuming.

Reversed-phase high-performance liquid chromatography (HPLC) has been used extensively [2,8,20–30]. It is an indirect method. To find an unknown log P_{ow}, a set of reference compounds of known log P_{ow} needs to be run under the same conditions. Calibration curves of log P_{ow} against retention time or capacity factors are used. The method preferably should be used for chemicals and reference compounds whose chemical structures do not differ significantly [31]. It can be used for a range of log P_{ow} from 0 to 6, is convenient, relatively fast, reproducible and less sensitive to impurities [8]. The disadvantages are that it is an indirect method, requires calibration and that occasional outliers occur [8].

Reversed-phase thin-layer chromatography (RP-TLC), also an indirect method, has been used [2,13,32,33] and again reference compounds of known log P_{ow} must be run. It has a range of 0 to 12 and is fast but less reproducible than HPLC, has inferior resolution and is less accurate than the shake flask method [8].

In the slow stirring method [2,23,31,34] the water and octanol phases are equilibrated under conditions of slow stirring. The formation of emulsions can be prevented and a very high log P_{ow} can be measured [31]. The method is slow, 2–4 days for equilibration to be achieved but has high accuracy and good repoducibility.

Another technique used is the column generator method where log P_{ow} up to 8.5 can be measured [2]. It is a complex method which includes a generator column for the preparation of an equilibrated solution, an extractor column for the collection and concentration of these solutes and a HPLC system for the measurement of the collected material [35]. Although the column generator method is suitable for hydrophobic chemicals, the labour required in the method is an important disadvantage [31]. Centrifugal partition chromatography, a form of counter current chromatography has also been used [36,37]. It allows the direct measurement of log P_{ow} and the ease of automation and accuracy may make this a useful measurement technique in the future.

2.2. Calculation

The calculation of log P_{ow} based on substituent constants (π) has been described [3,4]. These constants can be used only when the log P_{ow} of a structurally similar parent compound is known and they are dependent on the positions of the substituents in the molecule [31].

Another method of calculation is based on the summation of molecular fragments [4,38]. It is limited by applicability of additivity and interaction rules and availability of fragment constants and is less accurate than the shake flask method [8].

These methods of calculation do not have a limit on the range of log P_{ow} values which can be found. They can give a useful approximation of the log P_{ow}.

A relationship between log P_{ow} and solubilities has been shown [39]. Solubility has been used to calculated log P_{ow} [23,33]. It is limited to com-

pounds with low solubilities in both solvents, is affected by impurities and has low accuracy. The solubilities of a compound in both solvents are often not available [8].

Detailed reviews of the methods for the determination of log P_{ow} have been written by several authors [2,8,31].

3. APPLICATION OF LOG P_{ow} FOR CHOOSING HPLC CONDITIONS FOR ANALYSIS

Details of the use of reversed-phase HPLC for the determination of low P_{ow} have been given by several authors [8,21–23,25–27,29,30,33,40]. Methanol–water has been used for the mobile phase with one use of ethanol–water [33] and one laboratory of 22 in an inter-laboratory comparison [30] used acetonitrile–water. Only two laboratories used elevated temperature [22,33] and solvent programming was used by two authors [22,26] as well as by 9 out of 22 laboratories in an inter-laboratory comparison [30]. Commercial reversed-phase C_{18} columns (10 μm, 250 mm length) have been used by most authors. The most common mobile phase was methanol–water (3:1) at a flow-rate of 1 ml/min at ambient temperature.

Two inter-laboratory comparisons have been carried out [8,30]. The reproducibility of HPLC for log P_{ow} was found to be slightly superior or equivalent to the shake-flask method while the log P_{ow} could be estimated to within ±1 log unit of the shake-flask value [8]. With the use of 22 collaborators [30] a validated list of reference compounds was established for use in the HPLC determination of unknown log P_{ow} values and it was found that the log P_{ow} could usually be determined with a deviation of less than 0.5 from the shake-flask value.

With the detailed information available for HPLC determinations of log P_{ow} values for particular compounds these conditions would also be applied for any compound with the same or similar log P_{ow}. Where HPLC conditions for a compound with a well established log P_{ow} are known but not necessarily used for log P_{ow} determinations, these conditions should also be suitable for other compounds with the same or similar log P_{ow}. Hence log P_{ow} could be used to predict useful operating HPLC conditions. It would be applicable to hydrophobic compounds but it may not apply to hydrophilic compounds with a log P_{ow} less than two. In these cases the retention times are short and hydrogen bonding effects would play an important part.

4. APPLICATION OF LOG P_{ow} IN ESTIMATING ENVIRONMENTAL BEHAVIOUR OF PESTICIDES

Since the use of log P_{ow} as a measure of hydrophobicity was developed [3] correlations between various combinations of partition coefficients have been published. The log P_{ow} value has come to represent the tendency of a chemical to partition itself between the organic and aqueous environmental compartments. It has been found to be related to water solubility, organic carbon–water partition coefficient and bioconcentration factors (BCF) [21].

Correlations have been found between log P_{ow} and the BCF in aquatic and terrestrial organisms [41], with the BCF in fish [23,28,42,43], and bioconcentration kinetics in fish [34,44]. Relationships have been found between log P_{ow}, soil sorption, water solubilities, BCF and the parachor [13]. The uptake of pesticides in worms [14] and also the BCF of chemicals by alga [45] have relationships with log P_{ow}. Solubilities have been correlated with log P_{ow} [7,39,46,47] as have solubilities and BCF [19,48,49]. A relationship has been established between log P_{ow} and toxicity [18] for six organophosphates and their corresponding oxygen analogs in adult, male mice.

5. DECIDING IF A PESTICIDE SHOULD BE CLASSIFIED AS FAT-SOLUBLE

Partition coefficients have been used to classify compounds. They have been used with the classification of chemical mobility in soil [21]. The relationship between various properties of neutral molecules has been classified according to their log P_{ow} values [13].

A connection between hydrophobicity or fat-solubility and partition coefficients has been developed [3] and log P_{ow} can be considered to be a quantitative measure of the hydrophobicity of a compound [35]. Compounds with high log P_{ow} such as DDT and dieldrin have been classified as lipophilic [43].

When residues of fat-soluble pesticides are present in animal commodities such as meat and milk, they exist almost exclusively in the fat fraction. In

TABLE 1

PARTITION COEFFICIENTS (*n*-OCTANOL–WATER) OF PESTICIDES

Compound	Log P_{ow}	Derivation	Ref.
Acrolein	0.90	Cited	39
Aldicarb	1.08	Measured, inversion	9
	1.57	Measured, inversion	13
	1.13	Measured, shake flask	7
Aldicarb sulfone	−0.57	Measured, inversion	13
Aldicarb sulphoxide	−1.0	?	32
Aldoxycarb	−0.57	Measured, RP-TLC	9
Aldrin	5.66	Calculated	41
	7.4	Measured, RP-TLC	13
	6.50	Measured, shake flask	31
Allethrin	5.0	?	32
Ametryn	3.07	Measured, HPLC	27
	3.07	Calculated	27
Aminocarb	1.73	Measured, shake flask	7
Amitrole	−0.87	Measured, inversion	11
Atraton	2.69	Measured, HPLC	27
	2.69	Calculated	27
Atrazine	2.40	Measured, HPLC	40
	2.21	Measured, HPLC	40
	2.64	Measured, shake flask	
	2.68	or	45
	2.75	Cited	
	2.61	Measured, HPLC	27
	2.61	Calculated	27
	2.75	Measured, RP-TLC	33
	2.47	Measured, HPLC	30
Azinphos ethyl	3.40	Measured, shake flask	7
Azinphos ethyl O-analogue	1.63	Measured, shake flask	7
Azinphos methyl	2.69	Measured, shake flask	7
Azinphos methyl O-analog	0.78	Measured, shake flask	7
Benalaxyl	3.4	Cited	53
Benomyl	2.12	Cited	15
α-BHC	3.81	Measured, shake flask	54
	3.78	Measured, slow stirring	31
β-BHC	3.80	Measured, shake flask	54
	3.84	Measured, slow stirring	31
γ-BHC (lindane)	3.72	Measured, shake flask	54
	3.72	Measured, shake flask	25
	3.66	Measured, shake flask	43
δ-BHC	4.14	Measured, shake flask	54
Bifenthrin	6.00	Cited	55
Bromophos	4.88	Measured, shake flask	7
	5.21	Measured, slow stirring	31
Bromophos ethyl	5.68	Measured, shake flask	7
	6.15	Measured, slow stirring	31
Camphechlor	5.50	Cited	39
Captafol	3.83	Measured, inversion	13
Captan	2.54	Measured, inversion	13
	2.35	Measured, inversion	13
Carbanolate	2.3	Measured, inversion	13
Carbaryl	2.34	Measured, shake flask	56
	2.32	Measured, inversion	13
	2.36	Measured, inversion	13
	2.31	Measured, shake flask	7
	2.29	Measured, shake flask	43

TABLE 1 *(continued)*

Compound	Log P_{ow}	Derivation	Ref.
Carbendazim	1.40	Measured, inversion	14
	1.52	Measured, inversion	15
Carbofuran	1.63	Measured, shake flask	7
Carbophenothion	5.12	Measured, shake flask	7
	5.66	Measured, slow stirring	31
Carbophenothion methyl	4.82	Measured, shake flask	7
Carboxin	2.14	Cited	4-536[a]
Chloramben methyl ester	2.8	Measured, inversion	13
Chlorbromuron	3.09	Measured, inversion	13
Chlordane	5.16	Calculated	41
	6.00	Measured, HPLC	28
α-Chlordane	6.00	Cited	39
	6.0	Cited	44
γ-Chlordane	6.0	Cited	44
Chlordimeform	2.89	Measured, shake flask	7
Chlorfenac methyl	3.8	Measured, inversion	13
Chlorfenvinphos	3.10	Measured, inversion	13
	3.23	Measured, inversion	14
	3.81	Measured, shake flask	7
	3.80	Measured, shake flask	25
	3.82	Measured, shake flask	8
Chloridazon	1.14	Measured, shake flask	27
	1.50	Measured, inversion	13
Chlornitrofen	3.67	Measured, shake flask	43
Chlorotoluron	2.41	measured, inversion	13
Chloroxon	1.83	Measured, shaking	18
Chloroxuron	3.7	Measured, inversion	13
Chlorpyrifos	5.11	Measured, shake flask	48
	4.96	Measured, shake flask	7
	5.2	Measured, shaking	19
	5.27	Measured, slow stirring	31
Chlorpyrifos methyl	4.31	Measured, shake flask	48
	4.30	Measured, shake flask	7
Chlorsulfuron	1.09 to −0.41 at pH 4.5-12.0	Measured, stirring	17
Chlorthion	3.45	Measured, shaking	18
	3.63	Measured, slow stirring	34
Clofentezine	2.18	Cited	55
	3.1	Cited	53
Clopyralid	1.76	Calculated	41
Cyanazine	1.8	Measured, HPLC	27
	1.66	Calculated	27
Cyanophos	2.71	Measured, slow stirring	34
Cycloheximide	0.55	Measured, inversion	13
Cyhexatin	5.39	Cited	41
Cypermethrin	4.47	Measured, shake flask	59
2,4 Dichlorophenoxyacetic acid (2,4-D)	2.90 (undissociated)	Measured, inversion	10
	−0.24 (dissociated)	Measured, inversion	10
	2.81	Measured, shake flask	16
2,4-D dimethylamine	0.65	Measured, HPLC	24
2,4-D octyl ester	5.86	Measured, HPLC	40
	6.71	Calculated	40
	6.89	Calculated	40

(Continued on p. 8)

TABLE 1 *(continued)*

Compound	Log P_{ow}	Derivation	Ref.
DDE	5.63	Measured, HPLC	21
p,p'-DDE	5.69	Measured, HPLC	22
	5.89	Measured, HPLC	40
	6.96	Measured, slow stirring	31
	5.69	Measured, HPLC	28
	6.09	Measured, HPLC	29
DDT	4.64	Measured, HPLC	21
	3.98	Measured, shake flask	60
	5.90	Measured, shake flask	8
	6.12	Measured, HPLC	8
	5.89	Measured, HPLC	30
o,p'-DDT	5.75	Measured, HPLC	28
p,p'-DDT	6.38	Measured, shake flask	46
	6.2	Measured, slow stirring	23
	6.19	Measured, shake flask	25
	6.91	Measured, slow stirring	31
Deet	2.02	Measured, HPLC	24
Demetonthiol	1.93	Measured, shake flask	58
Desethylatrazine	1.53	Calculated	27
	1.51	Measured, HPLC	27
Desisopropylatrazine	1.12	Calculated	27
	1.15	Measured, HPLC	27
Dialifos	4.69	Measured, shake flask	48
Diazinon	3.11	Measured, inversion	13
	3.81	Measured, shake flask	7
	3.14	Measured, shake flask	43
Diazoxon	2.07	Measured, shake flask	7
Dicapthon	3.44	Measured, shaking	18
	3.58	Measured, shake flask	48
	3.62	Measured, shake flask	7
	3.72	Measured, slow stirring	34
Dicapthoxon	1.84	Measured, shaking	18
Dichlofenthion	5.14	Measured, shake flask	48
3,4 Dichloroaniline	2.78	Measured, inversion	13
p-Dichlorobenzene	3.42	Measured, shake flask	2
	3.38	Measured, generator column	2
	3.44	Measured, slow stirring	2
2,4-Dichlorophenol	2.8	Measured, inversion	13
Dichlorvos	1.47	Measured, shake flask	7
Dieldrin	4.54	Measured, slow stirring	23
	4.32	Measured, shake flask	43
	5.40	Measured, slow stirring	31
Dimethoate	0.50	Measured, shake flask	58
	0.79	Measured, inversion	13
	0.78	Measured, shake flask	7
Diphenyl	3.63	Measured, shake flask	25
	4.00	Measured, slow stirring	31
	4.00	Measured, shake flask	2
	3.83	Measured, generator column	2
	4.01	Measured, slow stirring	2
	3.91	Measured, shake flask	8
Diquat dichloride	−3.55	Cited	4-921[a]
Disulfoton	4.02	Measured, shake flask	7
Disulfoton sulfone	1.87	Measured, shake flask	7
Disulfoton sulfoxide	1.73	Measured, shake flask	7
Diuron	2.68	Measured, inversion	13

TABLE 1 *(continued)*

Compound	Log P_{ow}	Derivation	Ref.
Dowco 275	3.51	Measured, inversion	13
2,2-DPA (Dalapon, 2,2-dichloropropionic acid)	0.78	Calculated or cited	41
Endrin	4.56	Measured, shake flask	25
	5.20	Measured, slow stirring	31
EPN (O-ethyl O-4-nitrophenyl phenylphosphonothioate)	3.85	Measured, shake flask	43
Ethion	5.07	Measured, shake flask	7
ETU (ethylene thiourea)	−0.66	Cited	6
Fenamiphos	3.18	Measured, inversion	13
	3.23	Measured, shake flask	7
Fenchlorphos	4.88	Measured, shake flask	48
	4.81	Measured, shake flask	7
	5.07	Measured, slow stirring	31
Fenitrooxon	1.69	Measured, shaking	18
Fenitrothion	3.38	Measured, shake flask	48
	3.30	Measured, shaking	18
	3.40	Measured, shake flask	7
	3.47	Measured, slow stirring	34
	3.44	Measured, shake flask	43
Fenobucarb	3.18	Measured, shake flask	43
Fenoprop	2.44	Cited	41
	3.86	Cited	39
Fenpropathrin	3.03	Measured, shake flask	59
Fensulfothion	2.23	Measured, shake flask	7
Fensulfothion sulfide	4.16	Measured, shake flask	7
Fensulfothion sulfone	2.56	Measured, shake flask	7
Fenthion	4.09	Measured, shake flask	7
	4.17	Measured, slow stirring	34
Fenuron	0.96	Measured, inversion	13
Fenvalerate	4.42	Measured, shake flask	59
	6.2	Measured, shaking	19
Flamprop	2.90 (undissociated)	Measured, inversion	10
	−0.40 (dissociated)	Measured, inversion	10
Flucythrinate	6.2	Measured, shaking	19
Fluometuron	2.42	Measured, inversion	13
Fluorodifen	4.4	Measured, inversion	13
Fluvalinate	>3.85	Cited	55
Fonofos	3.89	Measured, shake flask	7
Fonofos O-analogue	2.11	Measured, shake flask	7
Guazatine	−1.15 at pH 3	Cited	55
Haloxyfop	4.47	Cited	55
	3.52	Cited	61
Haloxyfop methyl ester	4.07	Cited	55
Hexachlorobenzene (HCB)	5.50	Measured, shake flask	46
	5.44	Measured, inversion	13
	6.18	Measured, shake flask	25
	5.47	Measured, shake flask	2
	5.47	Measured, generator column	2
	5.73	Measured, slow stirring	2
	5.66	Measured, shake flask	8
Heptachlor	5.38	Calculated	41
	5.27	Measured, HPLC	40
	6.06	Calculated	40
	5.44	Measured, HPLC	28

(Continued on p. 10)

TABLE 1 *(continued)*

Compound	Log P_{ow}	Derivation	Ref.
	5.5	Calculated	29
	5.58	Measured, HPLC	29
Heptachlor epoxide	5.40	Measured, HPLC	28
Hexythiazox	2.53	Cited	55
Hydramethylnone	2.31	Cited	55
Imazapyr	0.11	Cited	55
Imazaquin	0.34	Cited	55
3-Indoleacetic acid	1.41	Cited	4-505[a]
Iodofenphos	5.16	Measured, shake flask	7
Iprobenfos	3.21	Measured, shake flask	43
Isazofos	3.82	Calculated from solubilities	33
	3.82	Measured, RP-TLC and HPLC	33
Isofenphos	4.12	Measured, shake flask	7
Leptophos	6.31	Measured, shake flask	48
	5.88	Measured, shake flask	7
	4.32	Measured, shake flask	43
Leptophos O-analogue	4.58	Measured, shake flask	7
Linuron	2.76	Measured, inversion	13
Malathion	2.89	Measured, shake flask	48
	2.84	Measured, shake flask	7
	2.94	Measured, slow stirring	34
Maleic hydrazide	−0.63	Measured, inversion	10
Metalaxyl	1.27	Calculated from solubilities	33
	1.65	Measured, RP-TLC and HPLC	33
Metflurazon	2.67	Measured, shake flask	57
Methidathion	2.42	Measured, shake flask	7
Methiocarb	2.92	Measured, inversion	13
Methomyl	0.13	Measured, shake flask	7
Methoxychlor	3.31	Measured, shake flask	60
Metobromuron	2.38	Measured, inversion	13
Metolachlor	3.28	Calculated from solubilities	33
	3.13	Measured, RP-TLC and HPLC	33
Metoxuron	1.64	Measured, inversion	13
Metribuzin	1.70	Cited	45
Mirex	6.89	Measured, HPLC	28
Molinate	3.21	Measured, shake flask	43
Monolinuron	2.30	Measured, inversion	13
Monuron	1.98	Measured, inversion	13
Naled	1.38	Measured, shake flask	58
Naphthalene	3.36	Measured, inversion	13
	3.25	Measured, slow stirring	23
	3.28	Measured, shake flask	25
	3.31	Measured, shake flask	8
NIA 24 110 (5-benzylfur-3-ylmethyl-*trans*-(+)-3-cyclopentylidenemethyl-2,2-dimethylcyclopropanecarboxylate) (RU 11679)	7.14	?	32
Nitrapyrin	3.02	Measured, inversion	13
Norflurazon	2.30	Measured, shake flask	57
Oxamyl	−0.47	Measured, inversion	13
Oxycarboxin	0.9	Measured, inversion	13
Paclobutrazol	3.2	Cited	62
Paraquat di-iodide	−5.00	Cited	4-921[a]
Paraoxon	1.59	Measured, shake flask	58
	1.98	Measured, shake flask	7
Paraoxon methyl	1.28	Measured, shake flask	58
	1.21	Measured, shaking	18

TABLE 1 *(continued)*

Compound	Log P_{ow}	Derivation	Ref.
Parathion	2.15	Measured, shake flask	63
	3.93	Measured, inversion	13
	3.81	Measured, shake flask	48
	3.76	Measured, shake flask	7
Parathion amino	2.60	Measured, shake flask	7
Parathion methyl	2.04	Measured, shake flask	65
	2.99	Measured, shaking	18
	2.94	Measured, shake flask	7
	1.8	Measured, shaking	19
	3.04	Measured, slow stirring	34
Pentachlorophenol	5.01	Measured, HPLC	22
	3.69	Measured, shake flask or cited	45
	5.01	Measured, HPLC	28
Pentanochlor	3.7	Measured, inversion	13
Permethrin	6.6	Measured, calculated	13
	3.49	Measured, shake flask	59
	6.5	Measured, shaking	19
	5.84 (*trans*)	Measured, HPLC	26
	6.24 (*cis*)	Measured, HPLC	26
Phenothiazine	4.15	Cited	3
Phenoxyacetic acid	1.47	Calculated from solubilities	47
	1.52	Measured, HPLC	30
Phenthoate	3.96	Measured, slow stirring	34
	2.89	Measured, shake flask	43
o-Phenyl phenol	3.09	Cited	4-558[a]
Phorate	4.26	Measured, inversion	13
	3.83	Measured, shake flask	7
Phorate sulfone	1.99	Measured, shake flask	7
Phorate sulfoxide	1.78	Measured, shake flask	7
Phosalone	4.30	Measured, shake flask	48
	4.38	Measured, shake flask	7
Phosmet	2.83	Measured, shake flask	48
	2.78	Measured, shake flask	7
	2.81	Measured, slow stirring	34
Phoxim	4.39	Measured, shake flask	7
Picloram	0.30	Calculated	41
Picloram methyl ester	2.3	Measured, inversion	13
Pirimiphos ethyl	4.85	Measured, shake flask	7
Pirimiphos methyl	4.20	Measured, shake flask	7
PP450 (Flutriafol)	2.29	Measured, inversion	12
Profenofos	4.70	Calculated from solubilities	33
	4.70	Measured, RP-TLC and HPLC	33
Profluralin	6.34	Calculated from solubilities	33
	5.58	Measured, RP-TLC and HPLC	33
Prometon	3.1	Calculated	27
	2.99	Measured, HPLC	27
Prometryn	3.48	Calculated	27
	3.34	Measured, HPLC	27
Propanil	2.8	Measured, inversion	13
Propazine	3.02	Calculated	27
	2.91	Measured, HPLC	27
Propham	2.60	Measured, inversion	13
Propoxur	1.58	Measured, shake flask	56
	1.55	Measured, shake flask	7
Quintozene	4.22	Measured, shake flask	43
Resmethrin	6.14	?	32

(Continued on p. 12)

TABLE 1 *(continued)*

Compound	Log P_{ow}	Derivation	Ref.
Simazine	1.51	Measured, inversion	13
	2.06	Measured, HPLC	40
	1.96	Measured, HPLC	40
	2.2	Calculated	27
	2.26	Measured, HPLC	27
Simetryn	2.66	Calculated	27
	2.8	Measured, HPLC	26
Strychnine	1.93	Cited	4-505[a]
Swep	2.80	Cited	4-273[a]
2,4,5-Trichorophenoxyacetic acid (2,4,5-T)	0.60	Calculated	41
Trichloroacetic acid	1.33	Cited	64
	0.10	Cited	6
	1.96	Calculated	6
p,p-TDE	6.22	Measured, slow stirring	31
Temephos	5.96	Measured, shake flask	7
Terbufos	4.48	Measured, shake flask	7
Terbufos sulfone	2.48	Measured, shake flask	7
Terbufos sulfoxide	2.21	Measured, shake flask	7
Terbumeton	3.1	Calculated	27
	3.1	Measured, HPLC	27
Terbuthylazine	3.02	Calculated	27
	3.06	Measured, HPLC	27
Terbutryn	3.72	Calculated from solubilities	33
	3.74	Measured, RP-TLC and HPLC	33
	3.48	Calculated	27
	3.43	Measured, HPLC	27
Tetrachlorvinphos	3.53	Measured, shake flask	8
Tetramethrin	4.7	?	32
Thiazfluron	1.46	Calculated from solubilities	33
	1.85	Measured, RP-TLC and HPLC	33
Thiobencarb	3.4	Measured, shaking	19
	3.42	Measured, shake flask	43
Tolylfluanid	3.90	Cited	62
Triazophos	3.55	Measured, shake flask	7
Triadimefon	2.77	Measured, inversion	12
Trichlorfon	0.43	Measured, shake flask	7
Trichloronate	5.23	Measured, shake flask	7
2,4,6-Trichlorophenol	2.97	Measured, shake flask or calculated	45
Tridiphane	4.34	Cited	55
Trietazine	3.15	Calculated	27
	3.07	Measured, HPLC	27
Trifluralin	3.97	Measured, shake flask	43
Vinclozolin	3.0	Cited	53
Warfarin	0.05	Cited	4-883[a]
	2.72	Cited	4-883[a]

[a] The additional number with ref. 4 gives the actual number of the reference in that source.

the case of meat, the residues of pesticides defined as fat-soluble are reported in terms of their concentration in the fat, not in the whole meat.

Extending the use of log P_{ow} to classify pesticides as fat-soluble has been proposed [50]. The scheme put forward suggests for log $P_{ow} < 3$ pesticides would not be fat-soluble, log P_{ow} 3–4 is an overlapping region and for log $P_{ow} > 4$ pesticides would

be fat-soluble.

The organochlorine pesticides are defined as fat-soluble. Most have a log P_{OW} >5 (aldrin, chlordane, DDE, DDT, dieldrin, endrin, heptachlor). The isomers of 1,2,3,4,5,6-hexachlorocyclohexane (BHC) have a log P_{OW} in the range of 3–4 and methoxychlor has a value of 3.31. The pyrethroids, also defined as fat-soluble, cyfluthrin, fenvalerate and permethrin have log P_{OW} values >5 while cypermethrin has values >4.

Organophosphates such as chlorfenvinphos (log P_{OW} 3.10–3.82), diazinon (log P_{OW} 3.11–3.81), fenitrothion (log P_{OW} 3.30–3.47) and phenthoate (log P_{OW} 2.89–3.96) are designated as fat-soluble [51]. Methidathion (log P_{OW} 2.42) and phosmet (log P_{OW} 2.83, 2.75, 2.81) are also designated as fat-soluble but these are the only such examples. It is compounds such as the organophosphates, the BHC isomers and methoxychlor, which are designated as fat-soluble and have log P_{OW} values from 3 to 4, which cause an overlapping region instead of a definite boundary.

Some compounds have log P_{OW} >4 but are not designated as fat-soluble. Cyhexatin (log P_{OW} 5.39), disulfoton (log P_{OW} 4.02), phorate (log P_{OW} 3.83, 4.26), phosalone (log P_{OW} 4.30, 4.38), profenofos (log P_{OW} 4.70) and terbufos (log P_{OW} 4.88) come in this category. There are some compounds such as the polymeric dithiocarbamates which are poorly soluble in both octanol and water. In this case if the log P_{OW} is greater than four these compounds could not be considered as fat-soluble and the use of log P_{OW} to classify these pesticides as fat-soluble would not be suitable.

6. COMPILATION OF THE DATA

The log P_{OW} values of pesticides and some breakdown products, metabolites and analogs are summarised in Table I. For consistency the common names used have come from one source [52]. The method of determination has been given (HPLC, RP-TLC, shake-flask and also slow stirring, inversion and shaking where there has been a variation on the shake flask method). Where the values have been calculated from substituent constants or fragment constants they are noted as calculated; however, where they have been calculated from solubilities this has been stated. The additional number with ref. 4 gives the actual number of the reference in that source.

The shake-flask method or a variation of it has been the preferred source of the values in an attempt to give the most accurate and useful data. In some cases close agreement was not found in the values for particular compounds even with this method. When values derived from a direct method were not available values from all other sources have been given. It has been indicated [8] that the useful range of the shake-flask method is −2.5 to 4.5. Where shake-flask values above this level have been found those from the slow stirring method are also included and if these were not available HPLC values have also been given.

Values from the RP-HPLC and RP-TLC methods are not as accurate as those from the shake-flask method. The accuracy of the HPLC method was considered not to be satisfactory according to the ±10% of reliably measured log P_{OW} values criteria adopted by one author [23]. Calculation by summation of molecular fragments is less accurate than the shake-flask method [8] and calculation from solubilities in water and octanol has low accuracy [8].

Data from the HPLC and calculation methods would not be accurate enough for use in bioactivity modling using partition coefficients because of the potential compounding of errors. Some values have been cited without the original method but only where no other values were found.

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