Corrigendum

Plastic Packaging
Interactions with Food and Pharmaceuticals
Edited by Otto G. Piringer and Albert L. Baner
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Appendices

Plastic Packaging. Second Edition. Edited by O.G. Piringer and A.L. Baner

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Appendix I

Peter Mercea

This section reviews most of the literature on the kinetics of small organic compounds (migrants) in polyethylenes (PEs) and polypropylenes (PPs) samples. An attempt was made to avoid a selection of data based on subjective criteria as to the quality of the experimental methods and/or model used to describe the diffusion process. However, in cases where a larger number of data were available for one and the same migrant, only the more recent experiments were cited. Then data was collected from experimental reports, which can be considered to be relevant to the topic of migration from polymeric packaging into foods and/or food simulants. In this respect the tables given below do not report diffusion data in swollen polymers because such situations are not suitable for food packaging.

There are a series of problems involved in an attempt to compare and interpret experimentally determined diffusion coefficients, D_p, in polymers.

First, problems result from the complex physical and chemical interactions between the migrants and the host polymer matrix. It is well documented that these interactions have a significant influence on the magnitude of D_p.

Then, problems are generated by the dependence of the morphological character of the polymer matrix upon its physical and chemical as well as manufacturing history. The D_p of a given migrant also depends on the molecular type and morphology/structure, density, and crystallinity of the polymer.

D_p depend on the temperature, T, too. The rate of this dependence often changes when the polymer undergoes a transition from a rubbery to a glassy state.

It is well known that the magnitude of D_p are also influenced by the initial amount of the migrant, $c_{p,0}$, formulated into the polymeric sample. High $c_{p,0}$ may have a plasticizing effect, which strongly influences the properties of a polymer matrix.

At last but not at least the D_p of a certain migrant may be influenced by the experimental setup used. There are numerous reports of migration experiments in which the polymeric sample is immersed into a liquid/solvent. It is logical to assume that such a liquid/solvent – which usually has relatively small molecules – diffuses into the polymer during the migration experiment. This process may influence to a certain degree not only the free volume available for the diffusional motion of the migrant, but even influence the interactions between the migrants and the host polymer matrix.

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Thus, taking into account those mentioned above, the sometimes large spread of D_p values reported in this appendix for one and the same migrant should not be considered as unusual or incorrect.

The rationale for the format of the tables given in the Appendix is the following.

The first column of the tables lists the chemical name of the migrant, as given in the publication cited. Because of that sometimes for one and the same organic migrant more than one chemical name appears in the tables. In column two the molecular weight, M_w, of the migrant is given.

Columns three and four give information about the polymer; namely about its density, crystallinity and/or morphology. In the case of polypropylenes, PPs, there are a series of abbreviations for the type of polymer, namely:

aT – atactic PP,
iT – isotactic PP,
HO – homo polymer,
CO – copolymer,
BO – biaxially oriented PP
UO – uniaxially oriented PP and
SB – stereo block polymer,

Diffusion of a noninteracting migrant through an isotropic polymer matrix due to its random motion can be described by Fick's first law (Eq. 7.5) in which the rate constant D is defined as the diffusion coefficient. In the fifth column of the tables the diffusion coefficients, as reported in the cited publications, are given. There are several types of D_p, namely:

D – concentration independent average diffusion coefficient,
$D_{c\to 0}$ – diffusion coefficient at "zero" diffusant concentration,
$D_{g.c.}$ – diffusion coefficient determined from inverse gas chromatography, and
D_s – diffusion coefficient in a polymeric sample in contact with a solvent or food simulant.

The sixth column gives information about the single temperature, T (°C), at or temperature range in which the migration experiments were performed.

Columns 7 to 9 summarize the diffusion parameters for each migrant. In the seventh column the diffusion coefficients, units cm^2/s, are given. In order to make a comparison of the reported D values as easy as possible an attempt was made to give as many as possible D's for $T = 23\,^{\circ}C$ (room temperature). In some cases this was possible only by extrapolating D's from measurements made at lower or higher temperatures. These situations are marked with (*. In those cases where a citation at 23 °C was not possible D's at other T's were given and marked with (** – T corresponding to the temperature given in column 6 or at another temperature given in the superscript – (^{70} for example.

In most cases the dependence of the diffusion in polymers on temperature is of Arrhenius type and described by the equation

$$D = D_0 \exp(-E_d/RT)$$

Table AI.1 Diffusion data for low molecular weight organic substances in Low Density Polyethylene (LDPE) and Linear Low Density Polyethylene (LLDPE) (densities up to 0.930 g/cm^3 @ room temperature).

Diffusing Species		Polymer		Experiment		Diffusion parameters			Ref.
Name	Molec. weight M_w (g/mol)	Density @ (°C) ρ_P (g/cm^3)	Cristallinity (%)	Type of diffusion coefficient	Temp. range of experiment (°C)	Diffusion coefficient @ (23°C) D (cm^2/s)	Pre-exponential coefficient l_gD_0	Activation energy E_D (kJ/mol)	
Methane	16.0	0.894 (25)	29.0	D	15; 45	4.64e-7	1.421	43.94	[1]
Methane	16.0	0.914 (25)	43.0	D	5; 55	1.7e-7	1.282	45.62	[1]
Methane	16.0	0.916 (25)	54.0	D	15; 50	1.94e-7	0.556	46.86	[2]
Methane	16.0	0.915 (25)	44.0	D	5; 50	1.58e-7	1.546	47.30	[3]
Methane	16.0	0.918	45.0	$D_{c\to 0}$	5; 35	2.98e-7	1.226	43.93	[4]
Methane	16.0	0.920 (23)	–	D	35, 50	1.79e-7(*	−1.712	28.52	[5]
Methane	16.0	–	–	D	30	2.28e-7(**	–	–	[6]
Ethylene	28.1	0.918	45.0	$D_{c\to 0}$	5; 35	1.34e-7	3.913	61.11	[4]
Ethylene	28.1	0.918	45.0	D	5; 35	1.81e-7	5.191	67.62	[4]
Ethylene	28.1	0.923 (25)	48.0	D	23; 73	1.25e-7	0.01023	39.18	[7]
Ethylene	28.1	–	–	D	30	1.01e-7(**	–	–	[6]
Ethane	30.1	0.894 (25)	29.0	D	5; 55	2.1e-7	2.036	49.38	[1]
Ethane	30.1	0.914 (25)	43.0	D	5; 55	5.87e-8	2.222	53.57	[1]
Ethane	30.1	0.920 (23)	–	D	33; 48	9.3e-8(*	0.948	34.46	[5]
Ethane	30.1	0.918	48.0	D	−26; 25	7.9e-8	2.874	56.52	[8]
Ethane	30.1	0.910 (25)	–	D	0; 50	4.98e-8	2.101	53.29	[9]
Ethane	30.1	0.918 (25)	–	D	25; 50	4.8e-8(*	2.505	55.66	[9]
Ethane	30.1	0.921 (25)	–	D	25; 50	3.48e-8(*	3.194	60.36	[9]
Ethane	30.1	0.924 (25)	–	D	20; 60	5.38e-8	1.888	51.89	[10]
Ethane	30.1	0.916 (25)	–	D	25	5.4e-8(**	–	–	[11]
Ethane	30.1	–	–	D	30	6.6e-8(**	–	–	[6]

Table AI.1 *(Continued)*

Diffusing Species		Polymer		Experiment		Diffusion parameters			Ref.
Name	**Molec. weight M_w (g/mol)**	**Density @ (°C) ρ_P (g/cm^3)**	**Cristallinity (%)**	**Type of diffusion coefficient**	**Temp. range of experiment (°C)**	**Diffusion coefficient @ (23°C) D (cm^2/s)**	**Pre-exponential coefficient $l_g D_0$**	**Activation energy E_D (kJ/mol)**	
Methanol	32.0	0.918 (23)	–	D_s	23	4.8e-8	–	–	[12]
Methanol	32.0	0.917 (23)	–	D	23	1.94e-8	–	–	[13]
Methanol	32.0	0.920 (25)	50.0	D	15;35	1.6e-8	0.031	44.36	[14]
Methanol	32.0	0.919	–	D	30	3.3e-8(**	–	–	[15]
Allene	40.1	0.894 (25)	29.0	D	10; 50	2.74e-7	1.414	45.20	[1]
Allene	40.1	0.914 (25)	43.0	D	10; 50	9.16e-8	1.750	49.80	[1]
Propylene	42.1	0.894 (25)	29.0	D	10; 50	1.75e-7	1.737	48.13	[1]
Propylene	42.1	0.914 (25)	43.0	D	10; 50	5.0e-8	1.933	52.31	[1]
Propylene	42.1	0.920 (25)	–	D	0; 22	1.07e-7(*	−0.260	38.0	[16]
Propane	44.1	0.894 (25)	29.0	D	10; 50	1.04e-7	2.248	52.31	[1]
Propane	44.1	0.914 (25)	43.0	D	10; 50	2.76e-8	2.264	55.66	[1]
Propane	44.1	0.915 (25)	44.0	D	25; 55	2.1e-8(*	3.491	63.19	[3]
Propane	44.1	0.918	45.0	$D_{c\to 0}$	5; 35	5.2e-8	2.929	57.86	[4]
Propane	44.1	0.920	–	D	30: 48	1.98e-8(*	0.2735	45.20	[5]
Propane	44.1	0.920 (25)	–	D	0; 25	6.65e-8	−7.176	23.3	[16]
Propane	44.1	–	–	D	30	3.1e-8(**	–	–	[6]
Ethanol	46.1	–	–	$D_{c\to 0}$	49.1	2.7e-10(**	–	–	[17]
Propionitrile	55.1	–	–	D	25	5.0e-9(**	–	–	[18]
Isobutylene	56.1	0.922 (25)	60.0	D	−8; 30	4.0e-8	4.102	65.16	[19]
Isobutylene	56.1	0.922 (25)	60.0	$D_{c\to 0}$	−8; 30	2.6e-8	3.607	63.41	[19]
Acetone	58.1	–	–	D	25	7.0e-9(**	–	–	[18]
Butane	58.1	0.924 (25)	–	D	30; 60	4.2e-8(*	−0.4437	39.25	[10]
Butane	58.1	0.922 (25)	50.0	D	25	1.95e-8(**	–	–	[20]
Butane	58.1	0.924 (25)	51.0	D	25	1.4e-8(**	–	–	[20]
Neopentane	72.1	0.918 (25)	–	D	25; 50	1.6e-9(*	6.503	86.73	[9]

n-Pentane	72.1	0.918 (25)	–	D	25; 50	8.05^{e}-9$^{(*}$	4.836	73.27	[9]
n-Butylaldehyde	72.1	0.922 (25)	50.0	D	25	1.18^{e}-8$^{(**}$	–	–	[20]
n-Butylaldehyde	72.1	0.924 (25)	51.0	D	25	1.05e-8$^{(**}$	–	–	[20]
Butanal	72.1	0.919 (25)	–	D	25	2.8e-9$^{(**}$	–	–	[21]
Butylalcohol	74.1	0.922 (25)	50.0	D	25	1.08e-8$^{(**}$	–	–	[20]
Butylalcohol	74.1	0.922 (25)	51.0	D	25	9.0e-9$^{(**}$	–	–	[20]
Benzene	78.1	0.922 (25)	60.0	$D_{c\rightarrow 0}$	0	1.9e-9$^{(**}$	–	–	[19]
Benzene	78.1	–	70.0	$D_{c\rightarrow 0}$	25; 50	9.9^{e}-9$^{(*}$	3.375	64.45	[22]
Benzene	78.1	0.916 (25)	54.0	$D_{c\rightarrow 0}$	25; 45	1.08e-8$^{(*}$	3.841	66.90	[23]
Benzene	78.1	0.918 (25)	54.0	$D_{c\rightarrow 0}$	25	1.98e-8$^{(*}$	–	–	[24]
Benzene	78.1	0.920 (25)	45.0	$D_{c\rightarrow 0}$	30; 40	1.41e-8$^{(*}$	0.4730	47.16	[25]
Benzene	78.1	0.915 (23)	42.0	$D_{c\rightarrow 0}$	23	3.8e-9	–	–	[26]
Benzene	78.1	0.918 (25)	–	$D_{c\rightarrow 0}$	25; 45	1.05e-8$^{(*}$	4.603	71.30	[27]
Benzene	78.1	0.918 (25)	45.0	$D_{c\rightarrow 0}$	25	4.0e-9$^{(*}$	–	–	[28]
Benzene	78.1	0.916 (25)	–	$D_{c\rightarrow 0}$	25; 35	1.4e-9$^{(*}$	−3.309	31.34	[29]
Benzene	78.1	0.917 (25)	–	D_{gc}	25	8.2e-9$^{(**}$	–	–	[30]
Benzene	78.1	0.918 (25)	–	$D_{c\rightarrow 0}$	25	2.15e-8$^{(**}$	–	–	[31]
Benzene	78.1	0.921 (25)	–	$D_{c\rightarrow 0}$	25	1.48e-8$^{(**}$	–	–	[31]
Benzene	78.1	0.922 (25)	–	$D_{c\rightarrow c\rightarrow 0}$	15; 35	9.9e-9	2.187	57.75	[31]
Benzene	78.1	0.928 (25)	–	$D_{c\rightarrow 0}$	25	6.9e-9$^{(**}$	–	–	[31]
Benzene	78.1	0.916 (25)	–	$D_{c\rightarrow 0}$	25; 45	7.1e-8$^{(*}$	1.876	51.1	[32]
Dimethylsulfoxide (DMSO)	78.1	0.915 (25)	44.0	D	30; 45	2.9e-9$^{(*}$	1.768	58.35	[33]
2-Hexene	84.2	–	70.0	$D_{c\text{-}0}$	25; 50	7.1e-9$^{(*}$	1.452	54.40	[22]
Cyclohexane	84.2	–	70.0	$D_{c\text{-}0}$	25; 50	4.1e-9$^{(*}$	2.388	61.10	[22]
Cyclohexane	84.2	0.918 (25)	54.0	$D_{c\rightarrow 0}$	25	6.1e-9$^{(**}$	–	–	[24]
Cyclohexane	84.2	0.915 (23)	42.0	$D_{c\rightarrow c\rightarrow 0}$	23	2.0e-9	–	–	[26]
Cyclohexane	84.2	0.921 (25)	–	$D_{c\rightarrow c\rightarrow 0}$	15; 35	1.04^{e}-8	0.5264	48.20	[31]
Cyclohexane	84.2	0.922	–	$D_{c\rightarrow c\rightarrow 0}$	25; 30	1.8e-9$^{(*}$	4.848	77.00	[34]
Cyclohexane	84.2	0.922	–	D_{S}	40	3.4e-8$^{(**}$	–	–	[35]
Methylenechloride	84.9	0.912 (25)	47.0	$D_{c\rightarrow c\rightarrow 0}$	25	9.2e-8$^{(**}$	–	–	[36]
Methylenechloride	84.9	0.917 (25)	50.2	$D_{c\rightarrow 0}$	25	8.2e-8$^{(**}$	–	–	[36]

Table AI.1 *(Continued)*

Diffusing Species		Polymer		Experiment		Diffusion parameters			Ref.
Name	Molec. weight M_w (g/mol)	Density @ (°C) ρ_P (g/cm^3)	Cristallinity (%)	Type of diffusion coefficient	Temp. range of experiment (°C)	Diffusion coefficient @ (23°C) D (cm^2/s)	Pre-exponential coefficient l_gD_0	Activation energy E_D (kJ/mol)	
Methylenechloride	84.9	0.924 (25)	52.0	$D_{c\to c\to 0}$	25	7.0e-8(**	–	–	[36]
Methylenechloride	84.9	0.924 (25)	–	$D_{c\to c\to 0}$	25	7.1e-8(**	–	–	[37]
Pentanal	86.1	0.919 (25)	–	D	25	7.0e-9(**	–	–	[21]
n-Hexane	86.2	0.922 (25)	50.0	D	25	1.05e-8(**	–	–	[20]
n-Hexane	86.2	0.924 (25)	51.0	D	25	9.0e-9(**	–	–	[20]
n-Hexane	86.2	–	70.0	$D_{c\to c\to 0}$	25; 50	5.3e-9(*	3.249	65.29	[22]
n-Hexane	86.2	0.918 (25)	54.0	$D_{c\to c\to 0}$	25; 45	1.05e-8(*	3.563	65.40	[24]
n-Hexane	86.2	0.918 (25)	–	$D_{c\to c\to 0}$	25; 45	8.4e-9(*	2.706	61.10	[27]
n-Hexane	86.2	0.918 (25)	45.0	$D_{c\to c\to 0}$	25	3.0e-9(**	–	–	[28]
n-Hexane	86.2	0.918 (25)	–	$D_{c\to c\to 0}$	25; 35	1.4e-9(*	−5.034	21.71	[29]
n-Hexane	86.2	0.918 (25)	–	$D_{c\to c\to 0}$	25; 50	1.04e-8(*	2.703	60.56	[38]
n-Hexane	86.2	0.915 (25)	43.2	$D_{c\to c\to 0}$	25	1.32e-8(**	–	–	[39]
n-Hexane	86.2	0.928 (25)	51.7	$D_{c\to c\to 0}$	25	7.8e-9(**	–	–	[39]
n-Hexane	86.2	0.916 (25)	–	$D_{c\to c\to 0}$	25; 45	5.1e-8(*	4.240	65.4	[32]
3-Methylpentane	86.2	–	70.0	$D_{c\to c\to 0}$	25; 50	4.1e-9(*	2.547	61.94	[22]
Neohexane	86.2	–	70.0	$D_{c\to c\to 0}$	25; 50	2.8e-9(*	2.900	64.86	[22]
Tetrafluormethane	88.0	0.918 (25)	45.0	$D_{c\to c\to 0}$	20; 50	7.9e-9	3.043	63.15	[40]
Ethylacetate	88.1	0.922 (25)	50.0	D	25	5.3e-8(**	–	–	[20]
Ethylacetate	88.1	0.924 (25)	51.0	D	25	4.7e-8(**	–	–	[20]
Ethylacetate	88.1	0.906 (30)	35.8	D	30	3.0e-8(**	–	–	[41]
Ethylacetate	88.1	–	–	D	25	1.1e-8(**	–	–	[42]
p-Dioxane	88.1	–	70.0	$D_{c\to c\to 0}$	25; 50	4.1e-9(*	4.912	75.33	[22]
1-Pentanol	88.2	0.919 (25)	–	D	25	6.4e-9(**	–	–	[21]

2-Pentanol	88.2	0.919 (25)	–	D	25	9.7e-9(**	–	–	[23]
Toluene	92.1	0.918 (25)	54.0	$D_{c\to c\to 0}$	25; 45	1.43e-8(*	7.508	87.00	[24]
Toluene	92.1	0.920	45.0	$D_{c\to 0}$	30; 50	1.37e-8(*	1.604	53.64	[25]
Toluene	92.1	0.918 (30)	47.3	$D_{c\to c\to 0}$	30	4.1e-8(**	–	–	[43]
Toluene	92.1	0.919 (30)	48.0	$D_{c\to c\to 0}$	30	3.6e-8(**	–	–	[43]
Toluene	92.1	0.918 (30)	–	D	30	4.3e-8(**	–	–	[44]
Toluene	92.1	0.891 (70)	35.0	$D_{c\to c\to 0}$	70	5.22e-7(**	–	–	[45]
Toluene	92.1	0.910 (70)	45.0	$D_{c\to 0}$	70	3.42e-7(**	–	–	[45]
Toluene	92.1	0.918 (23)	40.6	D	30	2.13e-8(**	–	–	[46]
Toluene	92.1	0.916 (25)	–	$D_{c\to c\to 0}$	25; 45	6.3e-8(*	1.976	52.0	[32]
Phenole	94.1	0.918 (23)	–	D_s	23	4.5e-9	–	–	[12]
Methyl bromide	95.0	0.919 (25)	58.0	D	0; 30	6.05e-8	2.061	52.58	[19]
Methylcyclohexane	98.2	0.918 (23)	40.6	D	30	5.8e-9(**	–	–	[46]
n-Heptane	100.2	0.919	–	D	30	1.1e-8(**	–	–	[15]
n-Heptane	100.2	0.918	–	$D_{c\to c\to 0}$	25; 35	1.2e-9(*	−5.122	21.47	[29]
n-Heptane	100.2	0.922 (25)	–	$D_{c\to 0}$	25; 30	4.4e-9(*	2.480	61.38	[34]
n-Heptane	100.2	0.918	–	$D_{c\to 0}$	25; 50	9.0e-9(*	4.484	70.99	[38]
n-Heptane	100.2	0.918 (23)	40.6	D	30	7.9e-9(**	–	–	[46]
n-Heptane	100.2	0.922	–	D_S	40	2.4e-8(**	–	–	[35]
n-Heptane	100.2	0.922	–	D_S	40	6.0e-9(**	–	–	[35]
n-Heptane	100.2	0.916 (25)	–	$D_{c\to 0}$	25; 45	8.6e-9(*	4.622	71.9	[32]
n-Hexylaldehyde	100.2	0.922 (25)	50.0	D	25	8.0e-9(**	–	–	[20]
n-Hexylaldehyde	100.2	0.925 (25)	51.0	D	25	6.0e-9(**	–	–	[20]
cis-3-Hexen-1-ol	100.2	0.918 (23)	–	D_s	23	1.4e-8	–	–	[47]
Hexanal	100.2	0.919 (25)	–	D	25	3.0e-10(**	–	–	[21]
Ethylpropionate	102.1	–	–	$D_{c\to 0}$	30	1.22e-8(**	–	–	[48]
Hexylalcohol	102.2	0.922 (25)	50.0	D	25	7.0e-9(**	–	–	[20]
Hexylalcohol	102.2	0.924 (25)	51.0	D	25	5.0e-9(**	–	–	[20]
1-Hexanol	102.2	0.919 (25)	–	D	25	1.44e-8(**	–	–	[21]

Table AI.1 *(Continued)*

Diffusing Species		Polymer		Experiment		Diffusion parameters			Ref.
Name	Molec. weight M_w (g/mol)	Density @ (°C) ρ_P (g/cm^3)	Cristallinity (%)	Type of diffusion coefficient	Temp. range of experiment (°C)	Diffusion coefficient @ (23°C) D (cm^2/s)	Pre-exponential coefficient l_gD_0	Activation energy E_D (kJ/mol)	
2-Hexanol	102.2	0.919 (25)	–	D	25	4.05e-9(**	–	–	[21]
Hexylalcohol	102.2	0.922 (25)	–	D	25	6.0e-9(**	–	–	[20]
Hexylalcohol	102.2	0.924 (25)	–	D	25	5.0e-9(**	–	–	[20]
o-Xylene	106.2	0.918 (25)	–	$D_{c\to 0}$	25	9.4e-9(**	–	–	[24]
m-Xylene	106.2	0.918 (25)	–	$D_{c\to 0}$	25	1.46e-8(**	–	–	[24]
p-Xylene	106.2	0.918 (25)	–	$D_{c\to 0}$	25	1.57e-8(**	–	–	[24]
N-Methylaniline	107.1	0.924 (25)	–	D	50	4.2e-8(**	–	–	[49]
p-Cresole	108.1	0.918 (23)	–	D_s	23	2.3e-9	–	–	[12]
Anisole	108.1	0.918 (25)	42.0	D_s	25	1.8e-8(**	–	–	[50]
n-Octane	114.2	0.922 (25)	50.0	D	25	6.8e-9(**	–	–	[20]
n-Octane	114.2	0.924 (25)	51.0	D	25	6.0e-9(**	–	–	[20]
n-Octane	114.2	0.918	–	$D_{c\to 0}$	25; 50	7.1e-9(*	6.115	80.81	[38]
iso-Octane	114.2	0.918 (23)	40.6	D	30	5.2e-9(**	–	–	[46]
2,2,4-Trimethylpentane	114.2	0.918 (25)	–	$D_{c\to 0}$	25; 50	2.3e-9(*	6.113	83.59	[38]
2,2,4-Trimethylpentane (Isooctane)	114.2	0.922	–	D_S	40	5.2e-9(**	–	–	[35]
Ethylbutyrate	116.2	0.922 (25)	50.0	D	25	2.2e-8(**	–	–	[20]
Ethylbutyrate	116.2	0.924 (25)	51.0	D	25	1.75e-8(**	–	–	[20]
Ethylbutyrate	116.2	–	–	D	23	1.79e-8	–	–	[51]
Ethylbutyrate	116.2	–	–	D	20; 40	1.86e-8	−6.291	8.16	[52]
Ethylbutyrate	116.2	–	–	D	30	2.1e-8(**	–	–	[53]
Heptanol	116.2	0.918 (23)	–	D_s	23	5.3e-9	–	–	[54]
Heptanol	116.2	0.918 (23)	–	D_s	23	5.5e-9	–	–	[12]
1-Heptanol	116.2	0.919 (25)	–	D	25	4.9e-10(**	–	–	[20]

2-Heptanol	116.2	0.919 (25)	–	D	25	1.39e-9(**	–	–	[21]
2,3-Benzopyrole (Indole)	117.1	0.918 (23)	–	D_s	23	5.5e-9	–	–	[47]
Chlorophorm	119.4	0.918 (25)	50.0	$D_{c\rightarrow 0}$	25	1.78e-8(**	–	–	[24]
Phenylmethylketone (Acetophenone)	120.1	0.918 (23)	–	D_s	23	1.10e-8	–	–	[47]
Mesitylene	120.2	0.920 (25)	45.0	$D_{c\rightarrow 0}$	30; 50	7.4e-9(*	0.6019	49.47	[25]
n-Propylbenzene	120.2	0.920 (25)	45.0	$D_{c\rightarrow 0}$	30; 50	1.16e-8(*	1.083	51.10	[25]
N,N-Dimethylaniline (DMA)	121.2	0.920 (25)	50.0	D_s	15; 35	1.73e-8	−0.070	43.58	[14]
N,N-Dimethylaniline (DMA)	121.2	0.916 (25)	29.0	D	25	5.5e-9(**	–	–	[55]
N,N-Dimethylaniline (DMA)	121.2	0.917 (25)	31.0	D	25	8.7e-9(**	–	–	[55]
N,N-Dimethylaniline (DMA)	121.2	0.918 (25)	42.0	D	25	7.2e-9(**	–	–	[56]
N,N-Dimethylaniline (DMA)	121.2	0.918 (25)	42.0	D_s	25; 45	3.8e-9(*	3.934	69.99	[56]
N,N-Dimethylaniline (DMA)	121.2	0.920 (25)	50.0	D_s	15;34	7.41e-9	3.021	63.19	[56]
Cresylmethylether	122.2	0.918 (23)	–	D_s	23	1.2e-8	–	–	[47]
2-Phenylethylalcohol	122.2	0.918 (23)	–	D_s	23	4.3e-9	–	–	[47]
3-Octen-2-one (Methylheptenone)	126.2	0.918 (23)	–	D_s	23	7.3e-9	–	–	[47]
n-Octylaldehyde	128.2	0.922 (25)	50.0	D	25	4.3e-9(**	–	–	[20]
n-Octylaldehyde	128.2	0.924 (25)	51.0	D	25	4.0e-9(**	–	–	[20]
Octanal	128.2	0.919 (25)	–	D	25	9.0e-11(**	–	–	[21]
n-Octanal (Aldehyde C_8)	128.2	0.918 (23)	–	D_s	23	2.3e-9	–	–	[47]
Octanal	128.2	–	–	D	20: 40	5.4e-9	−4.312	22.39	[52]
Ethylvalerate	130.2	–	–	$D_{c\rightarrow 0}$	30	1.0e-8(**	–	–	[48]
Octylalcohol	130.2	0.922 (25)	–	D	25	4.7e-9(**	–	–	[20]
Octylalcohol	130.2	0.924 (25)	–	D	25	4.0e-9(**	–	–	[20]
Amylaceticester (Isoamylacetate)	130.2	0.918 (23)	–	D_s	23	7.7e-9	–	–	[47]
p-isopropyltoluene (*p*-Cymene)	134.2	0.918 (23)	–	D_s	23	5.4e-9	–	–	[47]
2-(2-Ethoxyethoxy) ethanol	134.2	0.918 (23)	–	D_s	23	3.8e-9	–	–	[47]
n-Butylbenzene	134.2	0.920 (25)	45.0	$D_{c\rightarrow 0}$	30; 60	6.4e-9(*	0.514	49.33	[25]

Table AI.1 *(Continued)*

Diffusing Species		Polymer		Experiment		Diffusion parameters			Ref.
Name	Molec. weight M_w (g/mol)	Density @ (°C) ρ_P (g/cm^3)	Cristallinity (%)	Type of diffusion coefficient	Temp. range of experiment (°C)	Diffusion coefficient @ (23°C) D (cm^2/s)	Pre-exponential coefficient $l_g D_0$	Activation energy E_D (kJ/mol)	
2,4,6 Trimethylphenol	136.2	0.918 (23)	–	D_s	23	2.3e-9	–	–	[12]
4-Isopropenyl-1-methyl-1-cyclohexene (Limonene)	136.2	0.918 (23)	–	D_s	23	4.3e-9	–	–	[47]
4-Isopropenyl-1-methyl-1-cyclohexene (Limonene)	136.2	0.923 (25)	50.4	D	25; 45	4.2e-10(*	−2.436	39.31	[57]
4-Isopropenyl-1-methyl-1-cyclohexene (Limonene)	136.2	0.930 (25)	55.3	D	25; 45	4.0e-10(*	−5.243	23.54	[57]
4-Isopropenyl-1-methyl-1-cyclohexene (Limonene)	136.2	–	–	$D_{c\to 0}$	23	5.71e-11	–	–	[51]
4-Isopropenyl-1-methyl-1-cyclohexene (Limonene)	136.2	–	–	D	20; 40	1.10e-8	−4.546	19.25	[52]
4-Isopropenyl-1-methyl-1-cyclohexene (Limonene)	136.2	–	–	D	23	1.85e-8	–	–	[58]
7-Methyl-3-methylene-1,6-octadiene (Myrcene)	136.2	0.918 (23)	–	D_s	23	7.0e-9	–	–	[47]
7-Methyl-3-methylene-1,6-octadiene (Myrcene)	136.2	–	–	D	20; 40	1.04e-8	−4.320	20.76	[52]
2-Methyl-benzoicacid (Phenylacetate)	136.2	0.918 (23)	–	D_s	23	2.5e-9	–	–	[47]
3-Phenyl-1-propanol	136.2	0.918 (23)	–	D_s	23	2.8e-9	–	–	[47]
2,6,6-Trimethylbicyclo (3,1,1) hept-2-ene (alpha-Pinene)	136.2	0.918 (23)	–	D_s	23	1.4e-9	–	–	[47]

2,6,6-Trimethylbicyclo (3,1,1) hept-2-ene (alpha-Pinene)	136.2	–	–	D	20; 40	2.18e-8	−4.169	19.79	[52]
2,6,6-Trimethylbicyclo (3,1,1) hept-2-ene (alpha-Pinene)	136.2	–	–	D	23	9.7e-9	–	–	[58]
6,6-Dimethyl-2-methylenebicyclo (3,1,1) heptan-ropinene (Beta-Pinene)	136.2	0.918 (23)	–	D_s	23	1.4e-9	–	–	[47]
3,7,7-Trimethyl-bicyclo[4.1.0] hept-2-ene (Carene)	136.2	–	–	D_s	23	1.0e-8	–	–	[47]
2,4-Dimethyl-3-cyclohexen-1-carboxyalde-hyde	138.2	0.918 (23)	–	D_s	23	1.1e-9	–	–	[47]
n-Nonanal (Aldehyde C_9)	142.2	0.918 (23)	–	D_s	23	1.8e-9	–	–	[47]
n-Decane	142.2	0.922 (25)	50.0	D	25	4.2e-9(**	–	–	[20]
n-Decane	142.2	0.924 (25)	51.0	D	25	3.7e-9(**	–	–	[20]
n-Decane	142.2	–	–	$D_{g.c.}$	30; 80	3.4e-9(*	−4.213	24.12	[30]
n-Decane	142.2	0.918 (25)	–	$D_{c\rightarrow 0}$	25; 50	3.6e-9(*	8.644	96.83	[28]
cis-3-Hexen-1-yl-acetate	142.2	0.918 (23)	–	D_s	23	9.3e-9	–	–	[47]
7-Methylchinoline	143.2	0.918 (23)	–	D_s	23	4.3e-9	–	–	[47]
Ethylhexanoate	144.2	0.922 (25)	–	D	25	9.0e-9(**	–	–	[20]
Ethylhexanoate	144.2	0.924 (25)	–	D	25	2.7e-9(**	–	–	[20]
Ethylhexanoate	144.2	–	–	$D_{c\rightarrow 0}$	30	8.1e-9(**	–	–	[48]
Nonanol	144.3	0.918 (23)	–	D_s	23	4.0e-9	–	–	[12]
1,2-Benzopyrone (Cumarin)	146.2	0.918 (23)	–	D_s	23	5.4e-9	–	–	[47]
1-Methoxy-4-(1-propenyl) benzene (Anethol)	148.2	0.918 (23)	–	D_s	23	5.0e-9	–	–	[47]
cis,trans 3,7-Dimethyl-2,6-octadien-1-nitrile (Citralva)	149.2	0.918 (23)	–	D_s	23	1.7e-9	–	–	[47]
N,N- Di-ethylaniline (DEA)	149.2	0.920 (25)	50.0	D_s	20; 39	2.1e-9	2.635	64.06	[59]
3,4-Methylen-dioxybenzaldehyde (Heliotropine)	150.1	0.918 (23)	–	D_s	23	8.7e-10	–	–	[47]

Table AI.1 *(Continued)*

Diffusing Species		Polymer		Experiment		Diffusion parameters			Ref.
Name	Molec. weight M_w (g/mol)	Density @ (°C) ρ_P (g/cm^3)	Cristallinity (%)	Type of diffusion coefficient	Temp. range of experiment (°C)	Diffusion coefficient @ (23°C) D (cm^2/s)	Pre-exponential coefficient l_gD_0	Activation energy E_D (kJ/mol)	
Benzylacetate	150.2	0.918 (23)	–	D_s	23	7.0e-9	–	–	[47]
2,3,5,6 Tetramethylphenol	150.2	0.918 (23)	–	D_s	23	1.6e-9	–	–	[12]
Dimethylbenzylcarbinol	150.2	0.918 (23)	–	D_s	23	7.5e-10	–	–	[47]
Ethylbenzoate	150.2	0.918 (23)	–	D_s	23	1.1e-9	–	–	[47]
cis,trans 3,7-Dimethyl-2, 6-octadienal (Citral)	152.2	0.918 (23)	–	D_s	23	3.6e-9	–	–	[47]
cis,trans 3,7-Dimethyl-2, 6-octadienal (Citral)	152.2	–	–	$D_{c\to 0}$	23	3.2e-11	–	–	[51]
cis,trans 3,7-Dimethyl-2, 6-octadienal (Citral)	152.2	–	–	D	20; 40	2.22e-9	−0.899	43.94	[52]
cis,trans 3,7-Dimethyl-2, 6-octadienal (Citral)	152.2	–	–	D	23	3.5e-9	–	–	[58]
1,7,7-Trimethyl- 2,2,1 heptane-2-one (Campher)	152.2	0.918 (23)	–	D_s	23	1.5e-9	–	–	[47]
Carbontetrachloride	153.8	0.919		D	30	6.9e-9(**	–	–	[15]
Carbontetrachloride	153.8	–	70.0	$D_{c\to 0}$	25; 50	2.9e-9(*	6.092	82.86	[22]
Carbontetrachloride	153.8	0.918 (25)	50.0	$D_{c\to 0}$	25	6.6e-9(**	–	–	[24]
Carbontetrachloride	153.8	0.918 (25)	45.0	$D_{c\to 0}$	25	8.0e-10(**	–	–	[28]
1,7,7-Trimethylbicyclo 2,2,1 heptane-2-one (Borneol)	154.2	0.918 (23)	–	D_s	23	4.8e-10	–	–	[47]
3,7-Dimethyl-6-octene-1-al (Citronellal)	154.2	0.918 (23)	–	D_s	23	1.0e-9	–	–	[47]
1,8 Epoxy-p-Mentone (Eukalyptol)	154.2	0.918 (23)	–	D_s	23	1.0 e-9	–	–	[47]

3,7-Dimethyl-1,6-octadiene-3-ylacetate (Linalool)	154.2	0.918 (23)	–	D_s	23	1.9e-9	–	–	[47]
3,7-Dimethyl-1, 6-octadiene-3-ylacetate (Linalool)	154.2	–	–	$D_{c\rightarrow 0}$	23	1.39e-11	–	–	[51]
3,7-Dimethyl-1,6-octadiene-3-ylacetate (Linalool)	154.2	–	–	D	20; 40	2.7e-9	−5.391	18.04	[52]
2-*cis*-3,7-Dimethyl-2, 6-octadiene-1-ole (Nerol)	154.2	0.918 (23)	–	D_s	23	2.1e-9	–	–	[47]
2-*trans*-3,7-dimethyl-2,6-octadiene-8-ole (Geraniol)	154.2	0.918 (23)	–	D_s	23	1.5e-9	–	–	[47]
2-Isopropyl-5-methylhexanone (Menthon)	154.2	0.918 (23)	–	D_s	23	2.1e-9	–	–	[47]
cis-2[2-Methyl-1-propenyl]-4-methyl-tetrahydropyran (Roseoxyde L)	154.2	0.918 (23)	–	D_s	23	3.1e-9	–	–	[47]
1-Methyl-4-isopropyl-1-cyclohene-1-ole (Terpineol)	154.2	0.918 (23)	–	D_s	23	2.2e-9	–	–	[47]
1-Methyl-4-isopropyl-1-cyclohene-1-ole (alpha-Terpineol)	154.2	–	–	D	20; 40	8.6e-10	0.418	53.73	[52]
n-Decylaldehyde	156.3	0.922 (25)	50.0	D	25	2.4e-9(**	–	–	[20]
n-Decylaldehyde	156.3	0.924 (25)	51.0	D	25	2.1e-9(**	–	–	[20]
3,7-Dimethyl-6-octene-1-ol (Citronellol)	156.3	0.918 (23)	–	D_s	23	2.6e-9	–	–	[47]
n-Decanal (Aldehyd C_{10})	156.3	0.918 (23)	–	D_s	23	1.4e-9	–	–	[47]
Decanal	156.3	0.919 (25)	–	D	25	1.6e-10(**	–	–	[21]
Undecane	156.3	0.918 (23)	–	D_S	23	9.0e-9	–	–	[54]
Undecane	156.3	–	39.0	D	40	1.66e-8(**	–	–	[60]
Undecane	156.3	–	44.0	D	40	1.9e-8(**	–	–	[60]
2,6-Dimethyl-7-octene-2-ol (Dihydromyrcenol)	156.3	0.918 (23)	–	D_s	23	1.5e-9	–	–	[47]

Table AI.1 *(Continued)*

Diffusing Species		Polymer		Experiment		Diffusion parameters			Ref.
Name	Molec. weight M_w (g/mol)	Density @ (°C) ρ_P (g/cm^3)	Cristallinity (%)	Type of diffusion coefficient	Temp. range of experiment (°C)	Diffusion coefficient @ (23°C) D (cm^2/s)	Pre-exponential coefficient l_gD_0	Activation energy E_D (kJ/mol)	
2-Isopropyl-5-methylcyclohexanole (Menthol)	156.3	0.918 (23)	–	D_s	23	1.2e-9	–	–	[47]
2-Mthoxynaphthalene (Yara Yara)	158.2	0.918 (23)	–	D_s	23	4.7e-9	–	–	[47]
Ethylheptanoate	158.2	–	–	$D_{c\to 0}$	30	6.9e-9(**	–	–	[48]
Decylalcohol	158.3	0.922 (25)	50.0	D	25	2.9e-9(**	–	–	[20]
Decylalcohol	158.3	0.924 (25)	51.0	D	25	2.2e-9(**	–	–	[20]
3,7-Dimethyl-1-octanol	158.3	0.918 (23)	–	D_s	23	9.2e-10	–	–	[47]
3,7-Dimethyl-octane-3-ol	158.3	0.918 (23)	–	D_s	23	1.3e-9	–	–	[47]
Diethylmalonate	160.2	0.918 (23)	–	D_s	23	4.4e-9	–	–	[47]
Dimethylphenylethylcarbinole	164.2	0.918 (23)	–	D_s	23	7.9e-10	–	–	[47]
Methoxy-4(2-propenyl)phenol (Eugenol)	164.2	0.918 (23)	–	D_s	23	2.6e-9	–	–	[47]
2-Methoxy-4-prophenylphenol (Isoeugenol)	164.2	0.918 (23)	–	D_s	23	1.55e-9	–	–	[47]
1-Phenylethylacetate (Styrolacetate)	164.2	0.918 (23)	–	D_s	23	2.9e-9	–	–	[47]
2-Phenylethylacetate	164.2	0.918 (23)	–	D_s	23	5.7e-9	–	–	[47]
n-Undecene-2-al (Aldehyd C_{11})	168.3	0.918 (23)	–	D_s	23	9.6e-10	–	–	[47]
cis-Undecene-8-al (Aldehyd C_{11} inter)	168.3	0.918 (23)	–	D_s	23	9.0e-10	–	–	[47]
Diphenylmethane	168.3	0.918 (23)	–	D_s	23	4.8e-9	–	–	[47]
Diphenyloxide	170.2	0.918 (23)	–	D_s	23	3.7e-9	–	–	[47]

Ethyloctanoate	170.3	0.922 (25)	50.0	D	25	3.2e-9(**	–	–	[20]
Ethyloctanoate	170.3	0.924 (25)	51.0	D	25	2.8e-9(**	–	–	[20]
n-Undecylaldehyde (Aldehyde C_{11})	170.3	0.918 (23)	–	D_s	23	1.0e-9	–	–	[47]
n-Dodecane	170.3	0.922 (25)	50.0	D	25	3.3e-9(**	–	–	[20]
n-Dodecane	170.3	0.924 (25)	51.0	D	25	2.9e-9(**	–	–	[20]
n-Dodecane	170.3	0.918 (23)	–	D_s	23	2.7e-9	–	–	[61]
Dodecane (Alcane C_{12})	170.3	0.918 (23)	–	D_s	6; 40	2.6e-9	4.729	75.45	[61]
Dodecane	170.3	–	39.0	D	40	1.86e-8(**	–	–	[60]
Dodecane	170.3	–	39.0	D	40	9.97e-9(**	–	–	[60]
Dodecane	170.3	–	44.0	D	40	1.23e-8(**	–	–	[60]
Dodecane	170.3	–	44.0	D	40	7.76e-9(**	–	–	[60]
2,4-Di-*t*-butylphenol	170.5	0.918 (23)	–	D_s	23	1.2e-10	–	–	[12]
2,6-Di-*t*-butylphenol	170.5	0.918 (23)	–	D_s	23	9.8e-10	–	–	[12]
Ethyl-Naphtylether (Bromelia)	172.2	0.918 (23)	–	D_s	23	3.9e-9	–	–	[47]
3,7-Dimethyl-8-hydroxyoctanal (Hydroxycitronellal)	172.3	0.918 (23)	–	D_s	23	5.5e-10	–	–	[47]
Methyleugenol	178.2	0.918 (23)	–	D_s	23	3.0e-9	–	–	[47]
2-Methoxy-4-propenylanisol (Methylisoeugenol)	178.2	0.918 (23)	–	D_s	23	2.6e-9	–	–	[47]
Butyrated hydroanisole (BHA)	180.2	0.912 (31)	–	D	31	3.4e-9(**	–	–	[62]
Butyrated hydroanisole (BHA)	180.2	0.927 (31)	–	D	31	3.8e-9(**	–	–	[62]
2-Methoxy-4-propenylanisol (Methylisoeugenol)	178.2	0.918 (23)	–	D_s	23	2.6e-9	–	–	[47]
Diphenylmethanone (Benzophenone)	182.2	0.918 (23)	–	D_s	23	4.9e-9	–	–	[47]
n-Dodecylaldehyde (Aldehyde C_{12})	184.3	0.918 (23)	–	D_s	23	1.9e-10	–	–	[47]
2-Methyl-undecanal (Aldehyde C_{12} MNA)	184.3	0.918 (23)	–	D_s	23	1.8e-10	–	–	[47]

Table AI.1 *(Continued)*

Diffusing Species		Polymer		Experiment		Diffusion parameters			Ref.
Name	**Molec. weight M_w (g/mol)**	**Density @ (°C) ρ_P (g/cm^3)**	**Cristallinity (%)**	**Type of diffusion coefficient**	**Temp. range of experiment (°C)**	**Diffusion coefficient @ (23°C) D (cm^2/s)**	**Pre-exponential coefficient l_gD_0**	**Activation energy E_D (kJ/mol)**	
n-Undecalacton (Aldehyde C_{14})	184.3	0.918 (23)	–	D_s	23	2.7e-10	–	–	[47]
n-Dodecylaldehyde	184.3	0.922 (25)	50.0	D	25	1.9e-9(**	–	–	[20]
n-Dodecylaldehyde	184.3	0.924 (25)	51.0	D	25	1.6e-9(**	–	–	[20]
Citronellylformiate	184.3	0.918 (23)	–	D_s	23	2.3e-9	–	–	[47]
Tridecane	184.4	–	39.0	D	40	1.6e-8(**	–	–	[60]
Tridecane	184.4	–	39.0	D	40	9.0e-9(**	–	–	[60]
Tridecane	184.4	–	44.0	D	40	1.86e-8(**	–	–	[60]
Tridecane	184.4	–	44.0	D	40	8.98e-9(**	–	–	[60]
2,6-Di-*t*-butyl-4-methylphenol	184.6	0.918 (23)	–	D_s	23	6.6e-10	–	–	[12]
Dodecanol	186.4	0.918 (23)	–	D_s	23	1.1e-9	–	–	[12]
3-Methoxy-4-hydroxy-benzaldehyde (Verdylacetate)	190.2	0.918 (23)	–	D_s	23	2.1e-9	–	–	[47]
2-Methyl-3-(4-isopropyl) phenylpropanal (Cyclamen aldehyde)	190.3	0.918 (23)	–	D_s	23	1.2e-9	–	–	[47]
Triisopropanolamine (TIPA)	191.0	0.920	–	D	40; 100	1.9e-10	5.52	86.4	[63]
Dimethylbenzylcarbinylacetate (DMBCA)	192.3	0.918 (23)	–	D_s	23	1.09e-8	–	–	[47]
4-[2,6,6-Trimethy-2-cyclohexene-1-yle]-3-butene-2-one (Ionone)	192.3	0.918 (23)	–	D_s	23	1.2e-9	–	–	[47]
Dimethylphthalate (DMP)	194.2	0.918 (23)	–	D_s	23	1.9e-9	–	–	[47]

Allyl-3-cyclohexylpropionate	196.3	0.918 (23)	–	D_s	23	2.4e-9	–	–	[47]
2,6-Dimethyl-2,6-octadiene-8-yl-acetate (Geranylacetate)	196.3	0.918 (23)	–	D_s	23	1.6e-9	–	–	[47]
1,7,7-Trimethylbicylo-1,2, 2-haphtanyl-2-acetate (Isobromylacetate)	196.3	0.918 (23)	–	D_s	23	2.3e-9	–	–	[47]
3,7-Dimethyl-1,6-octadiene-3-ylacetate (Linalylacetate)	196.3	0.918 (23)	–	D_s	23	1.2e-9	–	–	[47]
1-Methyl-4-isopropyl-1-cyclohexene-4-yl-acetate (Terpinylacetate)	196.3	0.918 (23)	–	D_s	23	1.2e-9	–	–	[47]
Tetradecane (Alcane C_{14})	198.4	0.918 (23)	–	D_s	23	2.5e-9	–	–	[61]
Tetradecane (Alcane C_{14})	198.4	0.918 (23)	–	D_s	6; 40	1.9e-9	4.282	73.70	[61]
3,7-Dimethyl-6-octene-1-ylacetate	198.3	0.918 (23)	–	D_s	23	2.9e-9	–	–	[47]
p-tert.-Butylcyclohexylacetate (Oriclene extra)	198.3	0.918 (23)	–	D_s	23	1.2e-9	–	–	[47]
Ethyldecanoate	200.3	0.922 (25)	50.0	D	25	2.1e-9(**	–	–	[20]
Ethyldecanoate	200.3	0.924 (25)	51.0	D	25	1.7e-9(**	–	–	[20]
Methylundecanoate	200.3	0.918	44.0	D	20; 70	1.18e-8	2.73	60.39	[64]
Amylcinnamicaldehyde	202.3	0.918 (23)	–	D_s	23	1.4e-9	–	–	[47]
3-[4-*tert.*-Buthylphenyl]-2-methylpropanale (Lilial)	204.3	0.918 (23)	–	D_s	23	1.4e-9	–	–	[47]
N,N-Di-*n*-Butyl-aniline (DBA)	205.3	0.920 (25)	50.0	D_s	24; 43	1.2e-9(*	0.8007	55.01	[59]
2,4-Di-*tert*-butylphenole	206.3	0.918 (23)	–	D_s	23	1.2e-10	–	–	[12]
2,6-Di-*tert*-butylphenole	206.3	0.918 (23)	–	D_s	23	9.8e-10	–	–	[12]
3-Methyl-3-phenylglycidate (Aldehyde C_{16})	206.3	0.918 (23)	–	D_s	23	2.2e-9	–	–	[47]
5- (2,6,6-Trimethyl-2-cyclohexene-1-yle)-3-methyl-3-butene-2-one (Methyljonone-alpha)	206.3	0.918 (23)	–	D_s	23	6.6e-10	–	–	[47]

Table AI.1 *(Continued)*

Diffusing Species		Polymer		Experiment		Diffusion parameters			Ref.
Name	**Molec. weight M_w (g/mol)**	**Density @ (°C) ρ_P (g/cm^3)**	**Cristallinity (%)**	**Type of diffusion coefficient**	**Temp. range of experiment (°C)**	**Diffusion coefficient @ (23°C) D (cm^2/s)**	**Pre-exponential coefficient l_gD_0**	**Activation energy E_D (kJ/mol)**	
4-(2,6,6-Trimethyl-2-cyclohexene-1-yle)-3-methyl-3-butene-2-one (Methyljonone-gamma)	206.3	0.918 (23)	–	D_s	23	8.6e-10	–	–	[47]
Iso-amylsalicilate	208.3	0.918 (23)	–	D_s	23	2.1e-9	–	–	[47]
4-[4-Methyl-4-hydroxyamyl]-3-cyclohexene-carboxaldehyde (Lyral)	210.3	0.918 (23)	–	D_s	23	1.2e-10	–	–	[47]
Benzylbenzoate	212.3	0.918 (23)	–	D_s	23	3.2e-9	–	–	[47]
Pentadecane	212.4	–	39.0	D	40	1.15e-8(**	–	–	[60]
Pentadecane	212.4	–	39.0	D	40	7.66e-9(**	–	–	[60]
Pentadecane	212.4	–	44.0	D	40	1.3e-8(**	–	–	[60]
Pentadecane	212.4	–	44.0	D	40	1.5e-8(**	–	–	[60]
2,4-Dihydroxybenzophenone	214.2	–	–	D	5;100	2.2e-10	2.995	71.67	[65]
2,4-Dihydroxybenzophenone	214.2	0.920 (25)	43.0	D	35; 75	3.7e-10(*	4.210	77.30	[66]
2,4-Dihydroxybenzophenone (DHB)	214.2	–	–	$D_{c\rightarrow 0}$	25	5.0e-10(**	–	–	[67]
Tetradecanol	214.4	0.918 (23)	–	D_s	23	8.2e-10	–	–	[12]
Methyl Laureate	214.4	0.918 (25)	44.0	D	20; 70	9.3e-10	3.760	66.83	[64]
2-Hexyl-3-phenylpropenal (Jasmonal)	216.3	0.918 (23)	–	D_s	23	1.6e-9	–	–	[47]
2,6-Di-*tert*-tbutyl-4-methylphenol	220.4	0.918 (23)	–	D_s	23	6.6e-10	–	–	[12]
2,6-Di-*tert*-butyl-4-methylphenol (BHT)	220.4	–	–	D	25	1.5e-9(**	–	–	[67]
2,6-Di-Tert-butyl-4-methylphenol (Ionol)	220.4	–	–	D	65; 95	1.7e-8(60	0.832	54.82	[68]
2,6-Di-*tert*-butyl-4-methylphenol (Ionol)	220.4	0.918 (25)	44.0	D	23; 74	8.1e-10	3.842	73.28	[69]

2,6-Di-*tert*-butyl-4-methylphenol (Ionol)	220.4	0.918 (25)	44.0	D	75; 90	3.45e-8[70]	9.260	109.8	[69]
2,6-Di-*tert*-butyl-4-methylphenol (BHT)	220.4	–	–	D	25	9.0e-10[**	–	–	[70]
2,6-Di-*tert*-butyl-4-methylphenol (BHT)	220.4	0.918 (25)	44.0	D	10; 50	1.0e-9	4.150	74.47	[71]
2,6-Di-*tert*-butyl-4-methylphenol (BHT)	220.4	0.920 (25)	45.0	D_s	5; 60	4.8e-10	5.902	86.23	[72]
2,6-Di-*tert*-butyl-4-methylphenol (BHT)	220.4	0.917	–	D_s	30: 60	1.2e-10[*	6.639	93.83	[73]
Hexadecane (Alcane C_{16})	226.4	0.918 (23)	–	D_s	6; 40	1.0e-9	4.773	78.01	[61]
Hexadecane (Alcane C_{16})	226.4	–	39.0	D	40	1.0e-8[**	–	–	[74]
Hexadecane (Alcane C_{16})	226.4	–	44.0	D	40	1.2e-8[**	–	–	[74]
2-Hydroxy-4-methoxybenzophenone (Chimasorb 90)	228.2	–	–	D	25	7.0e-9[**	–	–	[70]
Methyl Tridecanoate	228.4	0.918 (25)	44.0	D	20; 70	7.8e-9	4.350	70.60	[64]
Phenylethylphenylacetate	240.3	0.918 (23)	–	D_s	23	3.0e-9	–	–	[47]
Hexadecanol	242.3	0.918 (23)	–	D_s	23	6.4e-10	–	–	[12]
Heptadecane	240.4	–	39.0	D	40	9.6e-9[**	–	–	[74]
Heptadecane	240.4	–	44.0	D	40	8.3e-9[**	–	–	[74]
Methylmiristate	242.4	0.918 (25)	44.0	D	20; 70	6.3e-9	4.710	73.15	[64]
Nonane-1,3-dioldiacetate (Jasmelia)	244.3	0.918 (23)	–	D_s	23	8.2e-10	–	–	[47]
Triphenylmethane	244.3	–	–	D	40	3.85e-9[**	–	–	[60]
Triphenylmethane	244.3	–	–	D	40	1.52e-9[**	–	–	[60]
Methylmiristate	242.4	0.918 (25)	44.0	D	20; 70	6.3e-9	4.710	73.15	[64]
Hexadecanone	254.4	0.918 (25)	44.0	D	30; 45	2.8e-9[*	9.550	102.6	[64]
Hexadecanone	254.4	0.918 (25)	44.0	D	48; 70	3.68e-8[40	2.770	61.0	[64]
n-Octadecane (Alcane C_{18})	254.5	0.918 (23)	–	D_s	6; 40	9.5e-10	5.416	81.82	[61]
Octadecane	254.4	–	39.0	D	40	6.0e-9[**	–	–	[60]
Ostadecane	254.4	–	44.0	D	40	4.0e-9[**	–	–	[60]

Table AI.1 *(Continued)*

Diffusing Species		Polymer		Experiment		Diffusion parameters			Ref.
Name	Molec. weight M_w (g/mol)	Density @ (°C) ρ_P (g/cm^3)	Cristallinity (%)	Type of diffusion coefficient	Temp. range of experiment (°C)	Diffusion coefficient @ (23°C) D (cm^2/s)	Pre-exponential coefficient $l_g D_0$	Activation energy E_D (kJ/mol)	
n-Octadecane	254.4	0.917	–	D_s	30; 60	7.8e-10(*	5.678	83.80	[73]
n-Octadecane (Alcane C_{18})	254.4	0.917	–	D_s	30; 60	3.5e-10(*	3.034	70.74	[75]
n-Octadecane	254.4	0.914	–	D	40; 90	1.19e-8(*	1.491	53.3	[76]
n-Octadecane	254.4	0.917	–	D_s	30; 60	1.63e-10(*	0.389	57.67	[77]
2-Hydroxy-4-ethanediolbenzophenone	258.3	–	–	D	5;100	2.1e-10	2.949	71.56	[65]
1,3,4,6,7,8-hexahydro-4,6,6,7, 8,8-haxamethyl-cyclopenta-2-benzopyrane (Galaxolid)	258.4	0.918 (23)	–	D_s	23	4.4e-10	–	–	[47]
7-Acetyl-1,1,3,4,4,6-Hexamethyl-tetra-hydronaphgthaline (Tonalid)	258.4	0.918 (23)	–	D_s	23	3.8e-10	–	–	[47]
N,N=-Diphenyl-*p*-phenylene-diamine (DPPD)	260.3	–	–	D_s	22	8.7e-10(**	–	–	[78]
Cedrylacetate	264.4	0.918 (23)	–	D_s	23	4.1e-10	–	–	[47]
Trichlormethylphenylcarbinylacetate (Roseacetol)	267.5	0.918 (23)	–	D_s	23	8.2e-10	–	–	[47]
2,6-Dinitro-1-methyl-3-methoxy-4-*tert.*-butylbenzole (Moschus Ambrette)	268.3	0.918 (23)	–	D_s	23	7.4e-10	–	–	[47]
Tetramethylpentadecane	268.3	–	–	D	40	5.6e-9(**	–	–	[60]
Tetramethylpentadecane	268.3	–	–	D	40	3.7e-9(**	–	–	[60]
Dicumilperoxyde	270.2	0.929 (25)	32.0	D	40: 70	1.02e-8(30	12.45	124.4	[79]
Tetramethylpentadecane	270.2	0.929 (25)	32.0	D	70	3.2e-7(**	–	–	[80]
2-Hydroxy-4-*n*-butoxybenzophenone	270.3	–	59.0	D	70: 90	2.04e-8(70	2.763	68.63	[81]

Octadecanol	270.5	0.918 (23)	–	D_s	23	4.8e-10	–	–	[12]
Methyl Palmitate	270.5	0.918 (25)	44.0	D	30; 70	4.4e-9	4.410	72.36	[64]
Stearylalcohol	270.5	–	–	D	40	3.04e-9(**	–	–	[60]
Stearylalcohol	270.5	–	–	D	40	1.09e-9(**	–	–	[60]
Di-butyl-phthalate (DBP)	270.5	–	–	$D_{c\rightarrow 0}$	20; 40	1.8e-12	2.635	81.45	[82]
Trans-9-octanacide	282.5	0.918 (25)	44.0	D	20; 40	3.4e-10	13.14	128.1	[64]
Eicosane (Alcane C_{20})	282.6	0.918 (23)	–	D_s	6; 40	6.3e-10	6.306	87.88	[61]
Stearic Acid	284.3	0.918 (25)	44.0	D	40; 70	8.2e-10(40	7.530	96.38	[64]
Heptadecanoate	284.5	0.918 (25)	44.0	D	30; 80	3.1e-9(*	6.580	85.50	[64]
Methylester 3-(3,5-di-*tert.*-butyl-4-hydroxy-phenyl) propionic acid	292.2	0.918	48.0	D	30; 60	2.8e-10(*	5.803	87.00	[83]
2,6-Dinitro-3,5-dimethyl-1-acetyl-4-*tert.*-butylbenzene (Moschus Ketone)	294.3	0.918 (23)	–	D_s	23	3.5e-10	–	–	[47]
2,4,6-Trinitro-1,3-dimethyl-5-*tert.*-butylbenzene (Moschus Xylol)	297.3	0.918 (23)	–	D_s	23	5.7e-10	–	–	[47]
Metyl Stearate	298.5	0.918 (25)	44.0	D	20; 38	1.2e-9	13.940	129.5	[64]
Docosane (Alcane C_{22})	310.6	0.918 (23)	–	D_s	6; 40	3.5e-10	7.227	94.54	[61]
Docosane	310.6	–	39.0	D	40	1.35e-9(**	–	–	[60]
Docosane	310.6	–	44.0	D	40	9.6e-10(**	–	–	[60]
Methylnonadecanoate	312.5	0.918 (25)	44.0	D	20; 40	1.1e-9	12.091	119.4	[64]
2-(2-hydroxy-3-*t*-butyl-5-methylphenyl)-5-chloro-benztriazol (Tinuvin 326)	315.8	0.918 (23)	–	D_s	23	2.0e-10	–	–	[12]
Heptadecylbenzene	316.4	–	–	D	40	4.9e-9(**	–	–	[60]
Heptadecylbenzene	316.4	–	–	D	40	3.8e-9(**	–	–	[60]
Propylester 3(3,5-di-*tert.*-butyl-4-hydroxyphenyl) propionic acid	320.2	0.918	48.0	D	30; 60	2.3e-10(*	6.167	89.60	[83]
2-Hydroxy-4-octoxybenzophenone	326.4	–	–	D	5;100	5.1e-10	2.754	68.28	[65]
2-Hydroxy-4-octoxybenzophenone (HOB)	326.4	–	–	D	25	1.2e-9(**	–	–	[67]

Table AI.1 *(Continued)*

Diffusing Species		Polymer		Experiment		Diffusion parameters			Ref.
Name	Molec. weight M_w (g/mol)	Density @ (°C) ρ_P (g/cm^3)	Cristallinity (%)	Type of diffusion coefficient	Temp. range of experiment (°C)	Diffusion coefficient @ (23°C) D (cm^2/s)	Pre-exponential coefficient l_gD_0	Activation energy E_D (kJ/mol)	
2-Hydroxy-4-octoxybenzophenone (Cyasorb UV 531)	326.4	0.918 (25)	44.0	*D*	5; 40	1.1e-9	5.950	84.37	[69]
2-Hydroxy-4-*n*-octoxybenzophenone	326.4	–	59.0	*D*	70; 90	2.08e-8[70]	0.924	56.50	[81]
2-Hydroxy-4-octoxybenzophenone	326.4	0,919	43.0	*D*	35; 50	5.1e-10[30]	19.88	88.14	[84]
2-Hydroxy-4-octoxybenzophenone	326.4	0,919	43.0	*D*	60; 75	2.48e-8[60]	2.002	61.23	[84]
Methyl Eicosanate	326.5	0.918 (25)	44.0	*D*	20; 40	7.2e-10	11.77	118.5	[64]
Methyl Eicosanate	326.5	0.918 (25)	44.0	*D*	40; 80	1.37e-8[40]	5.221	78.4	[64]
Behenyl alcohol	326.6	–	–	*D*	40	2.2e-10[**]	–	–	[60]
2-Hydroxy-4-ethandiol-thioacetic acid ester	332.4	–	–	*D*	5; 100	6.7e-11	3.725	78.75	[65]
Tetracosane	338.7	–	39.0	*D*	40	9.9e-10[**]	–	–	[74]
Tetracosane	338.7	–	44.0	*D*	40	6.7e-10[**]	–	–	[74]
2-2-Methylene bis (4-methyl-6-*t*.-butylphenol) (Plastanox 2246)	340.4	0.918 (25)	44.0	*D*	10; 70	2.2e-10	8.240	101.4	[69]
2-Hydroxy- 4-ethandiol methylthioacetic acid ester	346.4	–	–	*D*	5; 100	9.0e-11	3.461	76.54	[65]
Methyl Docosanate	354.5	0.918 (25)	44.0	*D*	20; 40	3.3e-10	12.22	123.0	[64]
2(2-hydroxy-3-5-di-*tert*.-butyl-phenyl)-5-chloro-benzotriazole (Tinuvin 327)	357.5	0.918 (25)	44.0	*D*	5; 70	1.6e-10	6.770	93.83	[69]
4-,4'-thio-bis-(3-methyl-6*tert*-butylphenol)	358.0	0.917 (25)	48.0	*D*	45; 70	2.24e-9[40]	2.236	65.32	[85]
4-4-Thio-bis-(6-*t*.-butyl-metacresol) (Santonox)	358.5	0.918 (25)	44.0	*D*	10; 70	2.0e-10	5.84	88.09	[69]

4-4-Thio-bis-(6-*t.*-butyl-metacresol) (Santonox)	358.5	0.918 (25)	44.0	D	10	3.8e-11[(**	–	–	[86]
Hexylester of 3(3,5-di-*tert.*-butyl-4-hydroxyphenyl)	362.4	0.918	48.0	D	30; 60	6.6e-11[(*	10.45	116.9	[83]
N-amido bis(2,2,6,6-tertamethyl-4-piperidinyl)–β–amionpropioamide	366.6	0.921	0	D	49; 80	1.02e-8[(40	−1.60	38.30	[87]
2-2-Methylene-bis(4-ethyl-6-*t.*-butyl-phenol) (Plastanox 425)	368.5	0.918 (25)	44.0	D	5; 70	8.7e-11	8.89	107.4	[69]
Methyl Tricosanate	368.5	0.918 (25)	44.0	D	20; 40	1.5e-10	14.99	140.6	[64]
Methyl Tricosanate	368.5	0.918 (25)	44.0	D	42; 80	1.47e-8[(40	1.93	58.50	[64]
2-Hydroxy-4 ethandiol *t*-butylthioacetic acid ester	388.5	–	–	D	5; 100	8.0e-12	4.400	87.85	[65]
Di-octyl-phthalate (DOP)	390.6	–	–	$D_{c\rightarrow 0}$	20; 40	4.7e-13	18.66	175.6	[82]
Octacosane	394.6	–	39.0	D	40	2.46e-10[(**	–	–	[60]
Octacosane	394.6	–	44.0	D	40	1.41e-10[(**	–	–	[60]
2,2,6,6 -Tetramethyl-4-piperidinol (Dastib 845)	411.2	0.921	–	D	23	6.9e-10	–	–	[87]
2,2,6,6 -Tetramethyl-4-piperidinol (Dastib 845)	411.2	0.921	–	D_s	20; 40	1.04e-9	7.902	95.68	[88]
2,2,6,6 -Tetramethyl-4-piperidinol (Dastib 845)	411.2	0.917 (25)	23.0	D	25; 60	1.8e-10[(*	1.54	64.0	[69]
Squalane	422.6	–	–	D	40	1.46e-9[(**	–	–	[60]
Squalane	422.6	–	–	D	40	7.3e-10[(**	–	–	[60]
2-2-Methylene-bis-(4-methyl-6-methyl-cyclohexyl-phenole) (Novox WSP)	420.5	0.918 (25)	44.0	D	5; 70	6.3e-11	7.42	99.85	[69]
4-4-Methylene-bis-(2-6 di-*tert.* butyl-phenole) (Ionox 220)	424.5	0.918 (25)	44.0	D	5; 70	1.0e-10	7.96	101.8	[69]
2,5 di(5-*tert*-butyl-2-benzoxazolyl)-thiophene (Uvitex OB)	430.5	–	–	D_s	22	2.04e-10[(**	–	–	[78]

Table AI.1 *(Continued)*

Diffusing Species		Polymer		Experiment		Diffusion parameters			Ref.
Name	Molec. weight M_w (g/mol)	Density @ (°C) ρ_P (g/cm^3)	Cristallinity (%)	Type of diffusion coefficient	Temp. range of experiment (°C)	Diffusion coefficient @ (23°C) D (cm^2/s)	Pre-exponential coefficient l_gD_0	Activation energy E_D (kJ/mol)	
D,l-α-Tocopherol (Irganox E 201)	431.0	0.930	–	D	40	6.9e-10(**	–	–	[63]
3,5-di-*tert.*-butyl-4-hydroxy-benzoic acid-(2,4-di-*tert*-butyl-phenyl) ester (Tinuvin 120)	438.6	0.918 (23)	–	D_s	23	1.8e-11	–	–	[12]
Methyl Octacosanate	438.6	0.918 (25)	44.0	D	20; 40	3.0e-11	14.65	142.7	[64]
2-Hydroxy-4 ethandiol *n*-octylthioacetic acid ester	445.5	–	–	D	5;100	3.0e-11	1.611	68.92	[65]
Dodecylester- 3(3,5-di-*tert.*-butyl-4-hydroxyphenyl) propionic acid	446.3	0.918	48.0	D	30; 60	1.3e-10(*	6.891	95.06	[83]
n-Dotriacontane	450.9	0.917	–	D_s	30: 60	6.4e-12(*	12.69	135.32	[73]
bis[2,2,6,6-tetramethyl-4-piperidinyl]-sebacate (Tinuvin 770)	480.7	0.921	–	D_s	20; 40	5.4e-12	3.587	72.83	[88]
bis[2,2,6,6-tetramethyl-4-piperidinyl-1-oxy}-sebacate	511.3	0.917	23.0	D	40; 80	2.0e-9(40	6.840	93.10	[89]
1,1,3-tris(2-methyl-4-hydroxy-5-butyl phenyl) butane (Topanol)	512.6	0.918 (23)	–	D_s	23	5.4e-11	–	–	[12]
Didodecyl-3-3-thiodipropionate (DLTDP)	514.4	0.918 (25)	44.0	D	5; 40	5.3e-10	9.940	108.9	[69]
Didodecyl-3-3-thiodipropionate (DLTDP)	514.4	0.918 (25)	44.0	D	40; 70	5.5e-9(40	6.230	86.8	[69]
Didodecyl-3-3-thiodipropionate (DLTDP)	514.4	0.916 (25)	43.0	D	20; 50	2.0e-11	15.40	147.8	[90]

Octadecylester 3-(3,5-di-*tert*-butyl-4-hydroxyphenyl) propionate (Irganox 1076)	531.4	0.918 (25)	48.0	*D*	30; 60	6.6e-11(*	8.170	104.0	[83]
3-(3,5-di-*tert*-butyl-4-hydroxyphenyl) propionate (Irganox 1076)	531.4	0.918 (25)	44.0	*D*	5; 40	1.1e-10	9.15	108.2	[69]
3-(3,5-di-*tert*-butyl-4-hydroxyphenyl) propionate (Irganox 1076)	531.4	0.916 (25)	43.0	*D*	30; 50	8.0e-11(*	10.18	114.9	[90]
3-(3,5-di-*tert*-butyl-4-hydroxyphenyl) propionate (Irganox 1076)	531.4	0.924 (25)	48.0	*D*	30; 50	1.1e-11(*	14.71	145.5	[90]
3-(3,5-di-*tert*-butyl-4-hydroxyphenyl) propionate (Irganox 1076)	531.4	0.928 (25)	51.0	*D*	30; 50	5.2e-12(*	18.54	169.0	[90]
3-(3,5-di-*tert*-butyl-4-hydroxyphenyl) propionate (Irganox 1076)	531.4	–	40.5	*D*	25	1.1e-11(**	–	–	[91]
3-(3,5-di-*tert*-butyl-4-hydroxyphenyl) propionate (Irganox 1076)	531.4	0.900	–	D_S	30; 60	7.2e-11(*	5.58	113.0	[92]
3-(3,5-di-*tert*-butyl-4-hydroxyphenyl) propionate (Irganox 1076)	531.4	0.910	–	*D*	40	2.43e-11(**	–	–	[63]
3-(3,5-di-*tert*-butyl-4-hydroxyphenyl) propionate (Irganox 1076)	531.4	0.918	–	*D*	40	3.8e-10(*	–	–	[63]
1-1-3-tris(2-methyl-4-hydroxy-5-*tert*.-butyl-phenyl)butane (Topanol CA)	544.5	0.918	44.0	*D*	5; 70	7.8e-11	6.230	92.6	[69]
1-1-3-tris(2-methyl-4-hydroxy-5-*tert*.-butyl-phenyl)butane (Topanol CA)	544.5	–	40.5	*D*	25	1.8e-10(**	–	–	[91]
2-Hydroxy-4-ethandiol *n*-dodecylthioacetic acid ester	557.5	–	–	*D*	5;100	2.8e-11	1.807	70.01	[65]
2-Hydroxy-4-ethandiol *n*-octadecylthio acetic acid ester	585.5	–	–	*D*	5;100	1.8e-11	1.602	69.92	[65]
N,N -Dioctadecyl-aniline (DODA)	597.6	0.918 (25)	42.0	*D*	25; 45	1.5e-9(*	3.002	66.96	[56]
2,2-Thiodiethyl-bis-[3-(3,5-di-*tert*-butyl-4-hydroxy phenyl)-propionat] (Irganox 1035)	643.4	0.918 (25)	44.0	*D*	5; 40	5.8e-12	14.00	143.0	[69]

Table AI.1 *(Continued)*

Diffusing Species		Polymer		Experiment		Diffusion parameters			Ref.
Name	**Molec. weight M_w (g/mol)**	**Density @ (°C) ρ_P (g/cm^3)**	**Cristallinity (%)**	**Type of diffusion coefficient**	**Temp. range of experiment (°C)**	**Diffusion coefficient @ (23°C) D (cm^2/s)**	**Pre-exponential coefficient l_gD_0**	**Activation energy E_D (kJ/mol)**	
Phosphorous acid, tris((2,4-di-*tert*-butylphenyl)ester (Irgafos 168)	646.0	0.905	–	*D*	80	2.4e-8(**	–	–	[63]
Phosphorous acid, tris((2,4-di-*tert*-butylphenyl)ester (Irgafos 168)	646.0	0.918	–	*D*	80	1.1e-8(**	–	–	[63]
Phosphorous acid, tris ((2,4-di-*tert*-butylphenyl)ester (Irgafos 168)	646.0	0.903	–	*D*	23	2.0e-12	–	–	[92]
Docosanyl Docosanate	649.1	–	–	*D*	40; 80	1.8e-9(40	6.903	93.70	[93]
Distearyl-thio-dipropionate (DSTDP)	682.5	0.916 (25)	43.0	*D*	40; 80	4.0e-9(40	6.12	87.0	[90]
1-3-5-Trimethyl-2-4-6-tri (3-5-di-*tert*-butyl-4-hydroxy benzyl)benzene (Ionox 330)	774.6	0.918 (25)	44.0	*D*	5; 70	7.9e-11	6.43	93.7	[69]
1-3-5-Trimethyl-2-4-6-tris (3-5-di-*tert*-butyl-4-hydroxy benzyl)benzene (Irganox 1330)	775.0	0.918	–	*D*	40	8.9e-11(**	–	–	[63]
Terephthalate-2-2-methyleme-bis-(4-methyl-6-*tert*-butyl) phenole (HMP12)	810.6	0.918 (25)	44.0	*D*	5; 70	2.4e-12	16.78	160.9	[69]

Polymer of 2,2,4,4-tetramethyl-7-oxa-3,20-diaza- 20-(2,3-epoxypropyl)dispiro [5.1.11.2]-heneicosane -21-one (Hostavin N 30)	840.0	0.930	–	*D*	49	1.61e-10(**	–	–	[63]
Tertakis[3-(3,5-di-*tert*-butyl- 4-hydroxy-phenyl) propionyloxymethyl)- methane (Irganox 1010)	1177.8	0.918 (25)	44.0	*D*	5;70	3.7e-12	8.95	115.5	[69]
Tertakis[3-(3,5-di-*tert*-butyl- 4-hydroxy-phenyl) propionyloxymethyl)- methane (Irganox 1010)	1177.8	0.921 (23)	43.0	*D*	45;80	4.6e-11(40	11.46	130.6	[94]
Tertakis[3-(3,5-di-*tert*-butyl-4- hydroxy-phenyl) propionyloxymethyl)- methane (Irganox 1010)	1177.8	–	–	*D*	25	5.02e-12(**	–	–	[70]
Tertakis[3-(3,5-di-*tert*-butyl-4- hydroxy-phenyl) propionyloxymethyl)- methane (Irganox 1010)	1177.8	0.917 (23)	23.0	*D*	25	5.6e-11(**	–	–	[95]
Tertakis[3-(3,5-di-*tert*-butyl-4 -hydroxy-phenyl) propionyloxymethyl) - methane (Irganox 1010)	1177.8	0.922	45.0	D_S	49	1.56e-11(**	–	–	[96]

Table AI.2 Diffusion data for low molecular weight organic substances in Polyethylene (PE). Medium and High Density Polyethylene (MDPE & HDPE); Densities larger than 0,930 g/cm^3 at room temperature.

Diffusing Species		Polymer		Experiment		Diffusion parameters			Ref.
Name	Molec. weight M_w (g/mol)	Density @ (°C) ρ_P (g/cm^3)	Cristallinity (%)	Type of diffusion coefficient	Temp. range of experiment (°C)	Diffusion coefficient @ (23°C) D (cm^2/s)	Pre-exponential coefficient l_gD_0	Activation energy E_D (kJ/mol)	
Methane	16.0	0.964 (25)	73.0	D*D*	15; 55	5.06e-e−8	0.384	43.52	[1]
Methane	16.0	0.931 (25)	45.0	D	25; 50	2.28e-e−8(*	0.851	48.13	[3]
Methane	16.0	0.951 (25)	–	D	25	8.2e-e−8(**	–	–	[9]
Methane	16.0	–	–	D	15; 95	1.0e-e−7	−2.51	25.15	[97]
Methane	16.0	0.955	–	D	25; 50	9.34e-e−8(**	0.35	41.85	[98]
Ethane	30.1	0.964 (25)	73.0	D	5; 55	1.26e-e−8	1.333	52.31	[1]
Ethane	30.1	0.950 (25)	–	D	0; 50	1.8e-e−8	1.711	53.57	[9]
Ethane	30.1	0.951 (25)	–	D	−5; 50	2.72e-e−8	1.064	48.91	[9]
Ethane	30.1	0.963 (25)	–	D	25; 50	7.2e-e−9(*	3.803	67.68	[9]
Ethane	30.1	0.964 (25)	–	D	25; 50	9.3e-e−9(*	1.372	53.27	[9]
Ethane	30.1	0.941 (23)	–	D	23	3.4e-e−8	–	–	[99]
Ethane	30.1	0.954 (23)	–	D	23	2.1e-e−8	–	–	[99]
Ethane	30.1	0.964 (23)	–	D	23	1.35e-e−8	–	–	[99]
Ethane	30.1	0.973 (23)	–	D	23	1.55e-e−8	–	–	[99]
Ethane	30.1	0.952 (25)	67.5	D	25	1.83e-e−8(**	–	–	[100]
Ethane	30.1	0.955 (25)	71.8	D	25	1.63e-e−8(**	–	–	[100]
Ethane	30.1	0.969 (25)	79.2	D	25	1.16e-e−8(**	–	–	[100]
Ethane	30.1	0.939 (25)	–	D	43; 73	1.36e-e−7(40	0.233	39.74	[101]
Allene	40.1	0.964 (25)	73.0	D	5; 55	2.18e-e−8			[1]
Cyclopropane	42.1	0.965 (25)	–	D	30; 57	1.40e-e−8(*	2.260	57.33	[101]
Propylene	42.1	0.964 (25)	73.0	D	5; 55	9.2e-e−9	1.194	52.31	[1]

Propane	44.1	0.965 (25)	73.0	D	5; 50	4.2e-e−9	1.667	56.92	[1]
n-Butane	58.1	0.965 (25)	–	D	35; 50	8.9e-e−9(30	2.70	62.36	[101]
Butane	58.1	0.951 (25)	–	D	25	3.6e-e−9(**	–	–	[9]
Butane	58.1	0.935 (25)	59.0	D	25	1.0e-e−8(**	–	–	[20]
Butane	58.1	0.944 (25)	65.0	D	25	7.0e-e−9(**	–	–	[20]
Neopentane	72.1	0.951 (25)	–	D	35; 50	2.4e-e−9(30	0.845	54.91	[9]
Neopentane	72.1	0.967 (25)	–	D	50; 80	2.0e-e−9(40	5.900	87.47	[101]
n-Pentane	72.1	0.951 (25)	–	D	25; 50	2.7e-e−9(*	4.933	76.53	[9]
n-Butylaldehyde	72.1	0.935 (25)	59.0	D	25	6.4e-e−9(**	–	–	[20]
n-Butylaldehyde	72.1	0.944 (25)	65.0	D	25	4.4e-e−9(**	–	–	[20]
Butanal	72.1	0.939	–	D	25	3.6e-e−9(**	–	–	[21]
Butylalcohol	74.1	0.935 (25)	59.0	D	25	4.8e-e−9(**	–	–	[20]
Butylalcohol	74.1	0.944 (25)	65.0	D	25	2.5e-e−9(**	–	–	[20]
Benzene	78.1	–	90.0	D	23	4.0e–e−9	–	–	[102]
Benzene	78.1	0.940 (25)	35.0	D	20; 40	4.0e-e−9	4.059	70.58	[103]
Methylenechloride (Dichlormethane)	84.9	0.945 (25)	81.0	$D_c \rightarrow_0$	25	2.66e-e−8(**	–	–	[104]
Methylenechloride (Dichlormethane)	84.9	0.949 (25)	71.8	$D_c \rightarrow_0$	25	2.7e-e−8(**	–	–	[105]
Methylenechloride (Dichlormethane)	84.9	0.949 (20)	68.0	$D_c \rightarrow_0$	25; 55	9.9e-e−9(*	4.261	69.50	[106]
Pentanal	86.1	0.939 (25)	–	D	25	2.8e-e−9(**	–	–	[21]
n-Hexane	86.2	0.938 (25)	68.0	D	0	4.9e-e−9(**	–	–	[19]
n-Hexane	86.2	0.954 (25)	75.0	D	0	2.3e-e−9(*	–	–	[19]
n-Hexane	86.2	0.939 (25)	59.0	D	25	6.0e-e−9(**	–	–	[20]
n-Hexane	86.2	0.944 (25)	65.0	D	25	3.8e-e−9(*	–	–	[20]
n-Hexane	86.2	0.934 (25)	55.8	$D_c \rightarrow_0$	25	3.01e-e−9(**	–	–	[39]
n-Hexane	86.2	0.937 (25)	57.3	$D_c \rightarrow_0$	25	2.47e-e−9(**	–	–	[39]
n-Hexane	86.2	0.944 (25)	62.5	$D_c \rightarrow_0$	25	4.17e-e−9(**	–	–	[39]
n-Hexane	86.2	0.949 (25)	66.2	$D_c \rightarrow_0$	25	1.3e-e−9(**	–	–	[39]

Table AI.2 *(Continued)*

Diffusing Species		Polymer		Experiment		Diffusion parameters			Ref.
Name	Molec. weight M_w (g/mol)	Density @ (°C) ρ_P (g/cm^3)	Cristallinity (%)	Type of diffusion coefficient –	Temp. range of experiment (°C)	Diffusion coefficient @ (23°C) D (cm^2/s)	Pre-exponential coefficient l_gD_0	Activation energy E_D (kJ/mol)	
n-Hexane	86.2	0.963 (25)	74.9	$D_{c\to 0}$	25	1.43e-9(**	–	–	[39]
n-Hexane	86.2	0.989 (25)	92.8	$D_{c\to 0}$	25	1.4e-10(**	–	–	[39]
n-Hexane	86.2	0.992 (25)	94.8	$D_{c\to 0}$	25	8.4e-10(**	–	–	[39]
n-Hexane	86.2	–	90.0	D	23	3.0e-9	–	–	[102]
Ethylacetate	88.1	0.939 (25)	59.0	D	25	2.9e-9(**	–	–	[20]
Ethylacetate	88.1	0.944 (25)	65.0	D	25	2.0e-9(**	–	–	[20]
1-Pentanol	88.2	0.939 (25)	–	D	25	2.93e-9(**	–	–	[21]
2-Pentanol	88.2	0.939 (25)	–	D	25	2.53e-9(**	–	–	[21]
Toluene	92.1	0.932	57.0	$D_{c\to 0}$	30	2.3e-8(**	–	–	[43]
Toluene	92.1	0.941	63.0	$D_{c\to 0}$	30	1.2e-8(**	–	–	[43]
Toluene	92.1	0.954	71.6	$D_{c\to 0}$	30	1.0e-8(**	–	–	[43]
Toluene	92.1	0.956	72.9	$D_{c\to 0}$	30	6.1e-9(**	–	–	[43]
Toluene	92.1	0.948 (25)	70.0	$D_{c\to 0}$	70	9.2e-8(**	–	–	[45]
Toluene	92.1	–	–	$D_{c\to 0}$	30	4.2e-9(**	–	–	[107]
Toluene	92.1	–	–	$D_{c\to 0}$	30	3.4e-9(**	–	–	[107]
n-Hexylaldehyde	100.2	0.935 (25)	59.0	D	25	7.0e-9(**	–	–	[20]
n-Hexylaldehyde	100.2	0.944 (25)	65.0	D	25	2.85e-9(**	–	–	[20]
Hexanal	100.2	0.939 (25)	–	D	25	1.71e-9(**	–	–	[21]
cis-3-Hexene-1-ol	100.2	0.956 (23)	–	D_s	23	1.5e-9	–	–	[52]
n-Heptane	100.2	0.948 (25)	70.0	$D_{c\to 0}$	70	4.8e-8(**	–	–	[45]
Hexylalcohol	102.2	0.939 (25)	59.0	D	25	3.0e-9(**	–	–	[20]
Hexylalcohol	102.2	0.944 (25)	65.0	D	25	1.85e-9(**	–	–	[20]

1-Hexanol	102.2	0.939 (25)	–	D	25	1.12e-9(**	–	–	[21]
2-Hexanol	102.2	0.939 (25)	–	D	25	1.44e-9(**	–	–	[21]
p-Xylene	106.2	0.955 (25)	–	$D_{c\rightarrow 0}$	30	3.8e-9(**	–	–	[108]
n-Octane	114.2	0.939 (25)	59.0	D	25	3.4e-9(**	–	–	[20]
n-Octane	114.2	0.944 (25)	65.0	D	25	2.15e-9(**	–	–	[20]
n-Octane	114.2	0.937 (25)	–	D	4; 45	2.6e-9	5.535	79.97	[20]
Heptanal	114.2	0.939 (25)	–	D	25	7.9e-10(**	–	–	[21]
Ethylbutyrate	116.2	0.939 (25)	–	D	25	1.05e-8(**	–	–	[20]
Ethylbutyrate	116.2	0.944 (25)	–	D	25	8.9e-9(**	–	–	[20]
1-Heptanol	116.2	0.939 (25)	–	D	25	3.6e-10(**	–	–	[21]
2-Heptanol	116.2	0.939 (25)	–	D	25	7.7e-10(**	–	–	[21]
N,N-Dimethylaniline	121.2	0.945 (25)	71.9	D	25	1.68e-9(**	–	–	[55]
2-Phenylethylalcohol	122.2	0.956 (23)	–	D_s	23	2.3e-10	–	–	[54]
n-Octylaldehyde	128.2	0.939 (25)	59.0	D	25	2.0e-9(**	–	–	[20]
n-Octylaldehyde	128.2	0.944 (25)	65.0	D	25	1.75e-9(**	–	–	[20]
Octanal	128.2	0.939 (25)	–	D	25	3.1e-10(**	–	–	[21]
Octylalcohol	130.2	0.939 (25)	59.0	D	25	2.0e-9(**	–	–	[20]
Octylalcohol	130.2	0.944 (25)	65.0	D	25	1.35e-9(**	–	–	[20]
Amylaceticester (Isoamylacetate)	130.2	0.956 (23)	–	D_s	23	8.5e-10	–	–	[54]
Amylacetate (Isoamylacetate)	130.2	–	–	D	30	9.1e-9(**	–	–	[109]
Amylacetate (Isoamylacetate)	130.2	–	–	$D_{c\rightarrow 0}$	33	3.05e-9(**	–	–	[109]
4-Isopropenyl-1-methyl-1-cyclohexene(Limonene)	136.2	0.956 (23)	–	D_s	23	5.7e-10	–	–	[54]
4-Isopropenyl-1-methyl-1-cyclohexene(Limonene)	136.2	–	–	$D_{c\rightarrow 0}$	23	5.0e-10	–	–	[110]

Table AI.2 *(Continued)*

Diffusing Species		Polymer		Experiment		Diffusion parameters			Ref.
Name	Molec. weight M_w (g/mol)	Density @ (°C) ρ_P (g/cm^3)	Cristallinity (%)	Type of diffusion coefficient –	Temp. range of experiment (°C)	Diffusion coefficient @ (23°C) D (cm^2/s)	Pre-exponential coefficient l_gD_0	Activation energy E_D (kJ/mol)	
n-ecane	142.2	0.939 (25)	59.0	D	25	2.15e-9(**	–	–	[20]
n-Decane	142.2	0.944 (25)	65.0	D	25	1.4e-9(**	–	–	[20]
2-Methylnaphthalene	144.2	0.940 (25)	–	D	25	3.6e-9(**	–	–	[20]
Dimethylbenzylcarbinol	150.2	0.956 (23)	–	D_s	23	4.5e-11	–	–	[54]
1,7,7-Trimethyl-2,2,1 heptane-2-one (Campher)	152.2	0.956 (23)	–	D_s	23	2.2e-11	–	–	[54]
Carbontetrachloride	153.8	0.952 (25)	70.0	$D_{c\rightarrow 0}$	25; 65	4.6e-10(*	5.800	85.77	[28]
3,7-Dimethyl-6-octene-1-al (Citronellal)	154.2	0.956 (23)	–	D_s	23	5.3e-11	–	–	[54]
n-Decylaldehyde	156.3	0.939 (25)	59.0	D	25	1.35e-9(**	–	–	[20]
n-DDecylaldehyde	156.3	0.944 (25)	65.0	D	25	1.03e-9(**	–	–	[20]
Decanal	156.3	0.939 (25)	–	D	25	1.8e-10(**	–	–	[21]
Undecane	156.3	–	52.0	D	40	1.03e-8(**	–	–	[60]
2-Isopropyl-5-methylcyclohexanole (Menthol)	156.3	0.956 (23)	–	D_s	23	5.7e-11	–	–	[54]
Decylalcohol	158.3	0.939 (25)	59.0	D	25	1.5e-9(**	–	–	[20]
Decylalcohol	158.3	0.944 (25)	65.0	D	25	8.0e-10(**	–	–	[20]
Methoxy-4(2-propenyl) phenol (Eugenol)	164.2	0.956 (23)	–	D_s	23	1.3e-10	–	–	[54]
Tetrachlorethylene	165.8	0.945 (25)	68.0	$D_{c\rightarrow 0}$	25	9.0e-9(**	–	–	[111]

*D*iphenylmethane	168.3	0.956 (23)	–	D_s	23	3.5e-10	–	–	[54]
Diphenyloxide	170.2	0.956 (23)	–	D_s	23	3.9e-10	–	–	[54]
Ethyloctanoate	170.3	0.939 (25)	59.0	D	25	1.9e-9(**	–	–	[20]
Ethyloctanoate	170.3	0.944 (25)	65.0	D	25	1.6e-9(**	–	–	[20]
4-Hydroxyundecanlactonidacide	170.3	0.956 (23)	–	D_s	23	4.8e-11	–	–	[54]
n-Dodecane	170.3	0.939 (25)	59.0	D	25	1.7e-9(**	–	–	[20]
n-odecane	170.3	0.944 (25)	65.0	D	25	1.25e-9(**	–	–	[20]
Dn-Dodecane (Alcane C_{12})	170.3	0.956 (23)	–	D_s	23	6.4e-10	–	–	[61]
n-odecane	170.3	–	52.0	D	40	4.23e-9(**	–	–	[60]
2-*tert*-Butyl-4-Methoxy Phenol (BHA)	180.2	0.954 (25)	–	D	10; 50	3.55e-10	2.071	65.28	[112]
n-Dn-Dodecylaldehyde (Aldehyde C_{12})	184.3	0.939 (25)	59.0	D	25	7.3e-10(**	–	–	[20]
Tridecane	184.4	–	52.0	D	40	8.47e-9(**	–	–	[60]
3,7-Dimethyl-1, 6-octadien-3-ylacetate(Linalylacetate)	196.3	0.956 (23)	–	D_s	23	8.2e-11(*	–	–	[54]
Tetradecane (Alcane C_{14})	198.4	0.956 (23)	–	D_s	23	4.9e-10	–	–	[61]
Ethyldecanoate	200.3	0.939 (25)	59.0	D	25	1.4e-9(**	–	–	[20]
Ethyldecanoate	200.3	0.944 (25)	65.0	D	25	1.1e-9(**	–	–	[20]
Pentadecane	212.4	–	52.0	D	40	7.78e-9(**	–	–	[60]
2,4-Dihydroxybenzophenone	214.2	0.953	68.0	D	60; 75	7.83e-10(50	7.406	102.10	[66]
2,4-Dihydroxybenzophenone	214.2	0.959	72.0	D	43; 75	4.1e-10(40	6.184	93.32	[66]
2,4-Dihydroxybenzophenone	214.2	0.959	72.0	D_s	44	9.9e-11(**	–	–	[66]
2,6-Di-*tert*-butyl-4-methylphenol (BHT)	220.3	–	–	D	23	1.38e-10	–	–	[70]
2,6-Di-*tert*-butyl-4-methylphenol (BHT)	220.3	0.948 (25)	64.0	D_s	5; 60	2.7e-12	–11.88	175.80	[72]
2,6-Di-*tert*-butyl-4-methylphenol (BHT)	220.3	0.978	–	D_s	30: 60	4.0e-12(*	7.449	106.77	[73]

Table AI.2 *(Continued)*

Diffusing Species		Polymer		Experiment		Diffusion parameters			Ref.
Name	Molec. weight M_w (g/mol)	Density @ (°C) ρ_P (g/cm^3)	Cristallinity (%)	Type of diffusion coefficient –	Temp. range of experiment (°C)	Diffusion coefficient @ (23°C) D (cm^2/s)	Pre-exponential coefficient lgD_0	Activation energy E_D (kJ/mol)	
2,6-Di-*tert*-butyl-4-methylphenol (BHT)	220.3	0.978	–	D_s	30: 60	4.6e-12(*	6.768	102.60	[75]
2,6-Di-*tert*-butyl-4-methylphenol (BHT)	220.3	–	–	D_s	30; 60	4.8e-12(*	3.372	77.56	[75]
2,6-Di-*tert*-butyl-*p*-cresole	220.3	0.934	54.0	D	20; 80	1.33e-9	0.800	54.82	[113]
2,6-Di-*tert*-butyl-4-methylphenol (BHT)	220.3	0.964	–	D_s	40	1.0e-10(**	–	–	[114]
2,6-Di-*tert*-butyl-4-methylphenol (BHT)	220.3	0.947	63	D_s	4; 40	2.67e-12	15.361	152.7	[96]
2,6-Di-*tert*-butyl-4-methylphenol (BHT)	220.3	0.947	67	D_s	40	2.37e-11	–	–	[96]
2-(2′-hydroxy-5′-methyl-phenyl)-2H-benzotriazol	225.3	–	–	D	40	1.36e-9(**	–	–	[60]
Hexadecane (Alcane C_{16})	226.4	0.956 (23)	–	D_s	23	2.9e-10	–	–	[5]
Hexadecane	226.4	–	52.0	D	40	6.37e-9(**	–	–	[60]
Heptadecane	240.4	–	52.0	D	40	5.86e-9(**	–	–	[60]
Triphenylmethane	244.2	–	–	D	40	6.98e-10(**	–	–	[60]
n-Octadecane (Alcane C_{18})	254.5	0.956 (23)	–	D_s	23	1.9e-10	–	–	[61]
Octadecane	254.5	–	52.0	D	40	2.16e-9(**	–	–	[60]

n-Octadecane	254.5	0.978	–	D_s	24; 60	3.5e-11(*	9.466	112.86	[73]
n-Octadecane	254.5	0.978	–	D_s	30; 60	5.0e-11(*	7.519	100.15	[75]
n-Octadecane	254.5	0.978	–	D_s	30; 60	8.8e-11(*	7.029	96.79	[75]
n-Octadecane	254.5	0.978	–	D_s	30; 60	3.1e-10(*	–2.838	37.81	[77]
n-Octadecane	254.5	0.934	54.0	D	20; 100	1.4e-8	1.300	51.89	[113]
Tetramethylpentadecane	268.6	–	52.0	D	40	1.02e-9(**	–	–	[60]
Stearyl alcohol	270.3	–	52.0	D	40	8.19e-10(**	–	–	[60]
Eicosane (Alcane C_{20})	282.6	0.956 (23)	–	D_s	23	9.0e-11	–	–	[61]
Docosane (Alcane C_{22})	310.6	0.956 (23)	–	D_s	23	3.3e-11	–	–	[61]
Docosane	310.6	–	52.0	D	40	4.17e-10(**	–	–	[60]
Heptadecylbenzene	316.2	–	52.0	D	40	1.2e-9(**	–	–	[60]
2-Hydroxy-4-octoxybenzophenone	326.4	0.953	68.0	D	55; 75	6.6e-11(50	16.81	166.90	[84]
2-Hydroxy-4-octoxybenzophenone	326.4	0.959	72.0	D	55; 75	1.3e-11(40	14.98	155.00	[84]
Behenyl alcohol	326.4	–	52.0	D	40	1.69e-10(**	–	–	[60]
Tetracosane	338.6	–	52.0	D	40	5.27e-10(**	–	–	[60]
2-2-Methylene bis (4-methyl-6-*t*.-butyl phenol) (Plastanox 2246)	340.4	0.937 (25)	57.0	D	50; 80	3.4e-10(50	6.030	95.79	[90]
2-2-Methylene bis (4-methyl-6-*t*.-butyl phenol) (Plastanox 2246)	340.4	0.952 (25)	68.0	D	50; 80	4.8e-11(50	7.840	112.38	[90]
2-2-Methylene bis (4-methyl-6-*t*.-butyl phenol) (Plastanox 2246)	340.4	0.954 (25)	69.0	D	50; 80	6.2e-11(50	7.800	111.30	[90]
N-Octadecyl-1-diethanolamine (*N*-ode)	357.4	0.934 (25)	54.0	D	20; 78	2.6e-9	0.500	51.47	[113]
Lauryllaureate	369.6	0.964 (30)	72.1	D	85	9.0e-9(**	–	–	[115]

Table AI.2 *(Continued)*

Diffusing Species		Polymer		Experiment		Diffusion parameters			Ref.
Name	**Molec. weight M_w (g/mol)**	**Density @ (°C) ρ_P (g/cm^3)**	**Cristallinity (%)**	**Type of diffusion coefficient –**	**Temp. range of experiment (°C)**	**Diffusion coefficient @ (23°C) D (cm^2/s)**	**Pre-exponential coefficient l_gD_0**	**Activation energy E_D (kJ/mol)**	
Lauryllaureate	369.6	0.977 (30)	85.5	D	85	1.1e-8(**	–	–	[115]
Di-(2-ethylhexyl)-phthalate	390.6	–	52.0	D	40	1.36e-10(**	–	–	[60]
Di-octyl-phthalate (DOP)	390.6	–	–	D	70	1.6e-11(**	–	–	[82]
Squalane	422.7	–	52.0	D	40	3.45e-10(**	–	–	[60]
2,5-Bis-(5-*tert*-buthyl-benzoxazol-2-yl)-thiophene (Uvitex OB)	430.5	–	52.0	D	40	9.33e-11(**	–	–	[60]
1,1-Bis-(2-hydroxy-3, 5-di-*tert*-butylphenyl)ethane (Isonox 129)	439.0	0.949	–	D	40:100	1.7e-13(*	7.876	122.7	[63]
2,4,6-tris(*tert*-butyl)phenyl) 2 butyl-2-ethyl-1, 3-propanediol-phosphite (Ultranox 640)	450.0	0.950	–	D	40	1.9e-11(**	–	–	[63]
n-Dotriacontane	450.9	0.978	–	D_s	30: 60	2.9e-13(*	14.71	154.40	[73]
n-Dotriacontane	450.9	0.978	–	D_s	30; 60	6.4e-13(*	13.22	144.00	[75]
Sebaic acid, bis(2,2,6,6-tetramethyl-piperidyl)ester (Sanol LS-770)	481.0	–	–	D	40; 110	9.9e-13(*	6.471	104.8	[63]

2,2-Ethyldiene-bis(4,6-di-*tert*-butyl-phenyl) fluoro- phosphonite	487.0	–	–	D	40	4.1e-13(**	–	–	[63]
bis [2,2,6,6-tetramethyl-4-piperidinyl-1-oxy] sebacate	511.0	0.943	46.0	D	60; 100	7.4e-10(60	7.387	105.30	[89]
Didodecyl-3-3-thiodipropionate (DLTDP)	514.4	0.937	57.0	D	60; 90	2.5e-9(60	4.580	84.00	[90]
Didodecyl-3-3-thiodipropionate (DLTDP)	514.4	0.952	68.0	D	60; 90	1.2e-9(60	4.260	83.90	[90]
Didodecyl-3-3-thiodipropionate (DLTDP)	514.4	0.954	69.0	D	60; 90	1.2e-9(60	2.070	70.0	[90]
Didodecyl-3-3-thiodipropionate (DLTDP)	514.4	0.952	68.0	D	30; 60	7.5e-10(*	18.67	157.50	[90]
Phsophorous acid, bis (2,4-di-*tert*-butyl-6-methylphenyl)ethyl ester (Irgafos 38)	515.0	0.946	–	D	70	4.7e-10(*	–	–	[63]
Phsophorous acid, bis (2,4-di-*tert*-butyl-6-methylphenyl) ethyl ester (Irgafos 38)	515.0	0.950	–	D	40; 70	1.2e-13(*	10.272	131.5	[63]
3-(3,5-di-*tert*-butyl-4-hydroxyphenyl) propionate (Irganox 1076)	531.4	0.937 (25)	57.0	D	30; 50	1.9e-12(*	18.57	171.6	[90]
3-(3,5-di-*tert*-butyl-4-hydroxyphenyl) ropionate (Irganox 1076)	531.4	0.937 (25)	57.0	D	50; 90	3.5e-10(50	5.33	91.44	[90]
3-(3,5-di-*tert*-butyl-4-hydroxyphenyl) ropionate (Irganox 1076)	531.4	0.952 (25)	68.0	D	30; 50	8.0e-13(*	13.9	147.27	[90]

Table AI.2 *(Continued)*

Diffusing Species		Polymer		Experiment		Diffusion parameters			Ref.
Name	Molec. weight M_w (g/mol)	Density @ (°C) ρ_P (g/cm^3)	Cristallinity (%)	Type of diffusion coefficient –	Temp. range of experiment (°C)	Diffusion coefficient @ (23°C) D (cm^2/s)	Pre-exponential coefficient l_gD_0	Activation energy E_D (kJ/mol)	
3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)propionate (Irganox 1076)	531.4	0.952 (25)	68.0	D	50; 90	8.3e-11(50	6.550	102.82	[90]
3-(3,5-di-*tert*-butyl-4-hydroxyphenyl) ropionate (Irganox 1076)	531.4	0.954 (25)	69.0	D	30; 50	9.8e-13(*	18.24	171.42	[90]
3-(3,5-di-*tert*-butyl-4-hydroxyphenyl) ropionate (Irganox 1076)	531.4	0.954 (25)	69.0	D	50; 90	1.8e-10(50	4.44	87.67	[90]
3-(3,5-di-*tert*-butyl-4-hydroxyphenyl) ropionate (Irganox 1076)	531.4	0.963	65.0	D_s	50; 121	2.2e-11(50	9.568	125.1	[116]
3-(3,5-di-*tert*-butyl-4-hydroxyphenyl) ropionate (Irganox 1076)	531.4	0.963	65.0	D_s	49; 110	6.2e-12(40	7.819	114.0	[117]
3-(3,5-di-*tert*-butyl-4-hydroxyphenyl) ropionate (Irganox 1076)	531.4	0.963	65.0	D_s	77; 135	3.3e-11(70	10.330	130.1	[118]
3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)propionate (Irganox 1076)	531.4	0.948	–	D	40: 60	1.2e-12(*	10.403-	126.3	[63]

Amines bis(hydrogenated tallow alkyl) oxidized mixture	537.0	–	–	D	40	2.5e-12(**	–	–	[63]
1-1-3-tris(2-methyl-4-hydroxy-5-*tert*-butyl-phenyl) butane	544.5	0.934	54.0	D	56; 100	2.8e-9(50	–0.300	51.06	[113]
N,*N*′-bis(3-(3,5-di-*tert*-butyl-4-hydroxyphenyl) propionyl)-hydrazide (Irganox MD 1024)	553.0	0.962	–	D	40: 100	5.5e-16(*	12.678	155.0	[63]
N,*N*′-bis(3-(3,5-di-*tert*-butyl-4-hydroxyphenyl) propionyl)-hydrazide (Irganox MD 1024)	553.0	0.962	–	D	40: 100	8.4e-16(*	13.212	160.3	[63]
Bis(2,4, di-*tert*-butylphenyl) pentaerythritol duphosphite (Ultranox 626)	604.0	0.950	–	D	40	3.9e-13(**	_	–	[63]
Bis(2,4, di-*tert*-butylphenyl) pentaerythritol duphosphite (Ultranox 626)	604.0	0.950	–	D	40	1.6e-12(**			[63]
Phosphorous acid, tris((2,4-di-*tert*-butylphenyl)ester (Irgafos 168)	646.0	0.946	–	D	80	2.4e-9(**	–	–	[63]
Phosphorous acid, tris((2,4-di-*tert*-butylphenyl)ester (Irgafos 168)	646.0	0.948	–	D	60	4.3e-11(**	–	–	[63]
Docosanic acid docosanyl ester(Behenyl behenate)	649.1	0.964 (30)	72.1	D	85; 95	2.3e-9(80	2.601	75.95	[115]
Distearyl-thio-dipropionate (DSTDP)	682.5	0.937 (25)	57.0	D	60; 90	1.2e-9(50	7.15	99.31	[90]
Distearyl-thio-dipropionate (DSTDP)	682.5	0.952 (25)	68.0	D	30; 60	3.5e-12(*	20.94	183.55	[90]
Distearyl-thio-dipropionate (DSTDP)	682.5	0.952 (25)	68.0	D	60; 90	8.8e-10(50	3.90	80.10	[90]

Table AI.2 *(Continued)*

Diffusing Species		Polymer		Experiment		Diffusion parameters			Ref.
Name	Molec. weight M_w (g/mol)	Density @ (°C) ρ_P (g/cm^3)	Cristallinity (%)	Type of diffusion coefficient –	Temp. range of experiment (°C)	Diffusion coefficient @ (23°C) D (cm^2/s)	Pre-exponential coefficient I_gD_0	Activation energy E_D (kJ/mol)	
Distearyl-thio-dipropionate (DSTDP)	682.5	0.954 (25)	69.0	D	60; 90	7.2e-10(50	4.46	84.11	[90]
3,9-bis(2-(3-(*tert*-butyl-4hydroxy-5-mrthylphenyl)propionyloxy)-*tert*-butyl)-2,4,8,10-tetraoxaspiro [5,5]undeca y (Sumilizer GA 80)	741.0	0.950	–	D	49	2.3e-11(**	–	–	[63]
Polymer of 2,2,4,4-tetramethyl-7-oxa-3,20-diaza-20-(2,3-epoxypropyl)dispiro [5.1.11.2]-heneicosane-21-one (Hostavin N 30)	840.0	0.950	–	D	49	1.3e-13(**	–	–	[63]
Poly(6-(N-(2,2,6,6-tetramethyl-4-piperidinyl)-n-butylamino)-1, 3,5-triazine-2,4-diyl) (2,2,6, 6-*tert*-amethyl-4-piperidinyl)imono-1, 6-hexanediyl((2,2,6,6-*tert*-amethyl-4-piperidinyl)imino-α-(N,N,N, *N′*-tetrabutyl-*N‴*-(2,2,6, 6-*tert*-amethyl-4-piperidinyl)imino) (Chimasorb 2020)	1060	0.950	–	D	60	7.1e-12(**	–	–	[63]

Tetrakis[3-(3-5-di-*tert*-butyl-4-hydroxy-phenyl) propionyloxymethyl)-methane(Irganox 1010)	1177.8	0.963	65.0	D_s	50; 130	4.4e-13[50]	12.394	153.0	[116]
Tetrakis[3-(3-5-di-*tert*-butyl-4-hydroxy-phenyl) propionyloxymethyl)-methane(Irganox 1010)	1177.8	0.963	65.0	D	49; 135	1.8e-14[40]	13.98	166.0	[117]
Tetrakis[3-(3-5-di-*tert*-butyl-4-hydroxy-phenyl) propionyloxymethyl)-methane(Irganox 1010)	1177.8	0.963	–	D_s	49; 135	1.4e-13[40]	11.16	143.8	[119]
2,2,2-Nitrilo(triethyl-tris (3,3,5,5-tetra-*tert*-butyl-1, 1-biphenyl-2,2-diyl) phosphite (Irgafos 12)	1465.0	0.950	–	D	40: 100	1.5e-14[*	0.869	83.3	[63]

Table AI.3 Diffusion data for low molecular weight organic substances in various types of polypropylenes (PPs).

Diffusing Species		Polymer		Experiment		Diffusion parameters			References
Name	**Molecular weight M_w (g/mol)**	**Density (°C) ρ_P (g/cm^3)**	**Crystallinity & type (%)**	**Type of diffusion coefficient (–)**	**Temperature range of experiment (°C)**	**Diffusion coefficient @ (23°C) D (cm^2/s)**	**Pre-exponential coefficient l_gD_0 (–)**	**Activation energy E_D (kJ/mol)**	
Ethylene	28.1	0.892	64.0	D	25	4.5e−9(**	–	–	[120]
Ethylene	28.1	0.899	52.0	$D_{g.c.}$	80	2.2e−6(**	–	–	[121]
Ethylene	28.1	0.901	50.0	$D_{g.c.}$	80	6.0e−7(**	–	–	[121]
Methanol	32.0	–	BO	D	23	9.0e−12	–	–	[122]
Methanol	32.0	–	BO	D	23	4.0e−12	–	–	[123]
Propylene	28.1	0.899	52.0	$D_{g.c.}$	80	2.0e−6(**	–	–	[121]
Propylene	28.1	0.901	50.0	$D_{g.c.}$	80	3.0e−7(**	–	–	[121]
Ethanol	46.1	–	–	$D_{c\to 0}$	20	8.4e−10(**	–	–	[123]
Ethanol	46.1	–	–	D_s	10–25	3.8e−10	15.335	140.3	[124]
Acetone	58.1	–	–	D_s	10–25	3.5e−10	−8.572	4.99	[124]
Dimethyl carbinol (2-propanol)	60.1	0.902 (23)	HO	D_s	23	1.2e−11	–	–	[125]
Benzene	78.1	0.910 (25)	63.0	$D_{c\to 0}$	25	8.5e−10(**	–	–	[28]
Benzene	78.1	–	10.0 (aT)	$D_{c\to 0}$	15–40	7.2e−9	6.557	83.33	[126]
Dichloromethane	84.5	0.883	47.0 (iT)	$D_{c\to 0}$	25	2.2e−9(**	–	–	[127]
Methylene chloride	84.5	0.883	47.0 (iT)	$D_{c\to 0}$	25	2.4e−9(**	–	–	[128]
n-Hexane	86.2	0.910 (25)	63.0	$D_{c\to 0}$	25	6.0e−10(**	–	–	[28]
n-Hexane	86.2	–	43.0 (iT)	D_s	30–60	4.68e−8(*	2.136	53.64	[129]
Tetrafluoromethane	88.0	0.895 (25)	47.8 (iT)	D	40–70	5.1e−9(30	3.024	65.62	[130]
Tetrafluoromethane	88.0	0.915 (25)	73.0 (iT)	D	40–70	6.0e−9(30	3.155	65.97	[130]
Tetrafluoromethane	88.0	0.895 (25)	47.6 (iT)	D	40–70	4.3e−9(30	3.598	69.38	[130]
Tetrafluoromethane	88.0	0.914 (25)	72.5 (iT)	D	40–70	6.0e−9(30	2.659	62.56	[130]

Tetrafluoromethane	88.0	0.906 (25)	61.8 (iT)	D	40–70	4.3e−9[30]	3.348	67.95	[130]
Tetrafluoromethane	88.0	0.915 (25)	72.6 (iT)	D	40–70	6.7e−9[30]	3.297	66.55	[130]
Toluene	92.1	–	74.0 (iT)	$D_{c\to 0}$	0–50	1.2e−9	1.262	57.61	[131]
Toluene	92.1	0.904	64.0 (UO)	$D_{c\to 0}$	30	5.6e−10[**]	–	–	[132]
Toluene	92.1	0.916	–	$D_{c\to 0}$	30	2.8e−11[**]	–	–	[132]
Toluene	92.1	0.916	78.0 (OP)	$D_{c\to 0}$	30	9.7e−11[**]	–	–	[132]
Bis-(2-chloroethyl)-sulfide	96.5	0.889 (25)	60.3 (iT)	$D_{c\to 0}$	20–40	9.1e−11	6.657	94.60	[133]
Bis-(2-chloroethyl)-sulfide	96.5	0.889 (25)	60.3 (iT)	D	20–30	9.3e−11	6.394	93.07	[133]
Methylcyclohexane	98.2	–	74.0 (iT)	$D_{c\to 0}$	0–50	1.65e−10	3.683	76.3	[131]
Methyl methacrylate	100.1	0.897 (25)	56.9 (iT)	$D_{c\to 0}$	60	9.1e−9[**]	–	–	[134]
Methyl methacrylate	100.1	0.902 (25)	62.4 (iT)	$D_{c\to 0}$	60	7.7e−9[**]	–	–	[134]
Methyl methacrylate	100.1	0.904 (25)	65.2 (iT)	$D_{c\to 0}$	60	4.9e−9[**]	–	–	[134]
Methyl methacrylate	100.1	0.905 (25)	66.1 (iT)	$D_{c\to 0}$	60	2.8e−9[**]	–	–	[134]
Methyl methacrylate	100.1	0.907 (25)	68.0 (iT)	$D_{c\to 0}$	60	1.4e−9[**]	–	–	[134]
Methyl methacrylate	100.1	0.912 (25)	74.5 (iT)	$D_{c\to 0}$	60	8.8e−9[**]	–	–	[134]
Methyl methacrylate	100.1	0.913 (25)	75.4 (iT)	$D_{c\to 0}$	60	6.8e−9[**]	–	–	[134]
Methyl methacrylate	100.1	0.914 (25)	76.3 (iT)	$D_{c\to 0}$	60	3.2e−9[**]	–	–	[134]
Methyl methacrylate	100.1	0.915 (25)	77.3 (iT)	$D_{c\to 0}$	60	2.4e−9[**]	–	–	[134]
Methyl methacrylate	100.1	0.897 (25)	56.9 (iT)	D	20–60	5.6e−10	1.767	62.44	[134]
Methyl methacrylate	100.1	0.907 (25)	68.0 (iT)	D	20–60	6.4e−11	1.494	66.22	[134]
n-Heptane	100.2	–	74.0 (iT)	$D_{c\to 0}$	0–50	3.7e−10	3.841	75.2	[131]
cis-3-Hexen-1-ol	100.2	0.900 (23)	CO	D_s	23	1.7e−10	–	–	[54]
cis-3-Hexen-1-ol	100.2	0.902 (23)	HO	D_s	23	1.5e−10	–	–	[54]
cis-3-Hexen-1-ol	100.2	0.902 (23)	HO	D_s	23	1.2e−10	–	–	[125]
2-Phenylethyl alcohol	122.2	0.900 (23)	CO	D_s	23	2.6e−11	–	–	[54]
2-Phenylethyl alcohol	122.2	0.902 (23)	HO	D_s	23	1.7e−11	–	–	[54]
2-Phenylethyl alcohol	122.2	0.900 (23)	CO	D_s	23	1.6e−11	–	–	[54]
2-Phenylethyl alcohol	122.2	0.902 (23)	HO	D_s	23	1.3e−11	–	–	[54]
2-Phenylethyl alcohol	122.2	0.902 (23)	HO	D_s	23	8.9e−11	–	–	[125]
Amylaceticester (Isoamylacetate)	130.2	0.900 (23)	CO	D_s	23	6.8e−11	–	–	[54]

Table AI.3 *(Continued)*

Diffusing Species		Polymer		Experiment		Diffusion parameters			References
Name	Molecular weight M_w (g/mol)	Density (°C) ρ_P (g/cm^3)	Crystallinity & type (%)	Type of diffusion coefficient (–)	Temperature range of experiment (°C)	Diffusion coefficient @ (23°C) D (cm^2/s)	Pre-exponential coefficient $l_g D_0$ (–)	Activation energy E_D (kJ/mol)	
Amylaceticester (Isoamylacetate)	130.2	0.902 (23)	HO	D_s	23	3.8e−11	–	–	[54]
Amylaceticester (Isoamylacetate)	130.2	0.900 (23)	CO	D_s	23	4.5e−11	–	–	[54]
Amylaceticester (Isoamylacetate)	130.2	0.902 (23)	HO	D_s	23	2.4e−11	–	–	[54]
Amylaceticester (Isoamylacetate)	130.2	0.902 (23)	HO	D_s	23	3.0e−11	–	–	[125]
4-Isopropenyl-1-methyl-1-cyclohexene (Limonene)	136.2	0.902 (23)	HO	D_s	23	3.2e−11	–	–	[54]
4-Isopropenyl-1-methyl-1-cyclohexene (Limonene)	136.2	0.902 (23)	HO	D_s	23	2.5e−11	–	–	[125]
4-Isopropenyl-1-methyl-1-cyclohexene (Limonene)	136.2	0.902 (23)	HO	D_s	23	3.75e−12	–	–	[122]
4-Isopropenyl-1-methyl-1-cyclohexene (Limonene)	136.2	–	51.0	D	30	1.51e−9(**	–	–	[135]
4-Isopropenyl-1-methyl-1-cyclohexene (Limonene)	136.2	–	63.0 (UO)	D	30	1.7e−9(**	–	–	[135]
4-Isopropenyl-1-methyl-1-cyclohexene (Limonene)	136.2	–	66.0 (BO)	D	30	4.2e−10(**	–	–	[135]
4-Isopropenyl-1-methyl-1-cyclohexene (Limonene)	136.2	–	UO	$D_{c\to 0}$	24	3.0e−12(**	–	–	[136]
4-Isopropenyl-1-methyl-1-cyclohexene (Limonene)	136.2	–	UO	D	24	1.6e−10(**	–	–	[136]

Ethyleneglycolmonophenylether (EMPhE)	138.2	–	–	D_s	25–60	4.6e−12(*	11.715	130.6	[124]
n-Decane	142.3	–	iT	D	70–110	5.3e−9(70	3.644	78.28	[81]
Bis-(2-chloroethyl)-ether	143.0	–	UO	D	25–45	1.71e−9(*	−4.318	25.21	[137]
Bis-(2-chloroethyl)-ether	143.0	–	BO	D	25–45	2.9e−10(*	−4.994	25.76	[137]
Dimethylbenzylcarbinol	150.2	0.900 (23)	CO	D_s	23	9.2e−12	–	–	[54]
Dimethylbenzylcarbinol	150.2	0.902 (23)	HO	D_s	23	1.1e−11	–	–	[54]
Dimethylbenzycarbinol	150.2	0.900 (23)	CO	D_s	23	1.2e−11	–	–	[54]
1,7,7-Trimethylbicyclo [2.2.1]heptan-2-one (Camphor)	152.2	0.900 (23)	CO	D_s	23	4.4e−12	–	–	[54]
1,7,7-Trimethylbicyclo [2.2.1]heptan-2-one (Camphor)	152.2	0.902 (23)	HO	D_s	23	3.3e−12	–	–	[54]
1,7,7-Trimethylbicyclo [2.2.1]heptan-2-one (Camphor)	152.2	0.900 (23)	CO	D_s	23	7.1e−12	–	–	[54]
1,7,7-Trimethylbicyclo [2.2.1]heptan-2-one (Camphor)	152.2	0.902 (23)	HO	D_s	23	3.9e−12	–	–	[54]
1,7,7-Trimethylbicyclo [2.2.1]heptan-2-one (Camphor)	152.2	0.902 (23)	HO	D_s	23	2.4e−12	–	–	[125]
Carbon tetrachloride	153.8	0.910 (25)	63.0	$D_{c\to 0}$	25	2.0e−10(**	–	–	[28]
3,7-Dimethyl-6-octen-1-al (Citronellal)	154.2	0.900 (23)	CO	D_s	23	1.3e−11	–	–	[54]
3,7-Dimethyl-6-octen-1-al (Citronellal)	154.2	0.902 (23)	HO	D_s	23	7.1e−12	–	–	[54]
3,7-Dimethyl-6-octen-1-al (Citronellal)	154.2	0.902 (23)	HO	D_s	23	4.3e−12	–	–	[54]
3,7-Dimethyl-6-octen-1-ol (Citronellal)	156.3	0.902 (23)	HO	D_s	23	5.0e−12	–	–	[125]
2-Isopropyl-5-methyl-cyclohexanole (Menthol)	156.3	0.900 (23)	CO	D_s	23	6.6e−12	–	–	[54]
2-Isopropyl-5-methyl-cyclohexanole (Menthol)	156.3	0.902 (23)	HO	D_s	23	2.6e−12	–	–	[54]
2-Isopropyl-5-methyl-cyclohexanole (Menthol)	156.3	0.902 (23)	HO	D_s	23	1.3e−11	–	–	[125]
Undecane	156.3	–	37.0	D	40	2.12e−9(**	–	–	[60]

Table AI.3 *(Continued)*

Diffusing Species		Polymer		Experiment		Diffusion parameters			References
Name	**Molecular weight M_w (g/mol)**	**Density (°C) ρ_P (g/cm^3)**	**Crystallinity & type (%)**	**Type of diffusion coefficient (–)**	**Temperature range of experiment (°C)**	**Diffusion coefficient @ (23°C) D (cm^2/s)**	**Pre-exponential coefficient l_gD_0 (–)**	**Activation energy E_D (kJ/mol)**	
Methoxy-4(2-propenyl)phenol (Eugenol)	164.2	0.900 (23)	CO	D_s	23	2.4e−11	–	–	[54]
Methoxy-4(2-propenyl)phenol (Eugenol)	164.2	0.902 (23)	HO	D_s	23	1.5e−11	–	–	[54]
Methoxy-4(2-propenyl)phenol (Eugenol)	164.2	0.900 (23)	CO	D_s	23	2.1e−11	–	–	[54]
Methoxy-4(2-propenyl)phenol (Eugenol)	164.2	0.902 (23)	HO	D_s	23	1.05e−11	–	–	[125]
Diphenylmethane	168.3	0.900 (23)	CO	D_s	23	2.9e−11	–	–	[54]
Diphenylmethane	168.3	0.902 (23)	HO	D_s	23	1.6e−11	–	–	[54]
Diphenylmethane	168.3	0.900 (23)	CO	D_s	23	2.2e−11	–	–	[54]
Diphenylmethane	168.3	0.902 (23)	HO	D_s	23	1.5e−11	–	–	[54]
Diphenylmethane	168.3	0.902 (23)	HO	D_s	23	1.25e−11	–	–	[125]
Diphenylamine (DPA)	169.2	–	AT	$D_{c\rightarrow o}$	40–60	7.3e−10$^{(40}$	18.88	168.0	[138]
Diphenylamine (DPA)	169.2	–	AT	D	40–60	5.1e−9$^{(40}$	5.73	84.0	[138]
Diphenyl oxide	170.2	0.900 (23)	CO	D_s	23	3.8e−11	–	–	[54]
Diphenyl oxide	170.2	0.902 (23)	HO	D_s	23	2.0e−11	–	–	[54]
Diphenyl oxide	170.2	0.900 (23)	CO	D_s	23	2.1e−11	–	–	[54]
Diphenyl oxide	170.2	0.902 (23)	HO	D_s	23	1.3e−11	–	–	[54]
Diphenyl oxide	170.2	0.902 (23)	HO	D_s	23	1.8e−11	–	–	[125]
n-Dodecane (Alcane C_{12})	170.3	0.900 (23)	CO	D_s	23	1.1e−10	–	–	[61]
n-Dodecane (Alcane C_{12})	170.3	0.902 (23)	HO	D_s	23	5.9e−11	–	–	[61]
Dodecane	170.3	–	37.0	D	40	9.34e−10$^{(**}$	–	–	[60]
γ-Undecanlactone	184.3	0.902 (23)	HO	D_s	23	7.0e−12	–	–	[125]
Tridecane	184.3	–	37.0	D	40	1.12e−9$^{(**}$	–	–	[60]

Methyl decanoate	186.3	–	64.0 (HO)	D	50–100	1.17e−11[40]	11.27	133.0	[139]
Methyl decanoate	186.3	–	64.0 (HO)	D	50–100	1.35e−11[40]	10.614	128.7	[139]
4-Ethoxybenzoic acid, ethyl ester	194.0	–	–	D	40–70	9.1e−11[*	8.132	103.0	[63]
4-Ethoxybenzoic acid, ethyl ester	194.0	–	–	D	40–70	1.2e−10[*	6.548	93.3	[63]
4-Ethoxybenzoic acid, ethyl ester	194.0	–	–	D	40–70	6.1e−11[*	6.239	93.3	[63]
3,7-Dimethyl-1,6-octadien-3-yl acetate (Linalyl acetate)	196.3	0.900 (23)	CO	D_s	23	1.4e−10	–	–	[54]
3,7-Dimethyl-1,6-octadien-3-yl acetate (Linalyl acetate)	196.3	0.902 (23)	HO	D_s	23	7.8e−12	–	–	[54]
3,7-Dimethyl-1,6-octadien-3-yl acetate (Linalyl acetate)	196.3	0.900 (23)	CO	D_s	23	1.2e−11	–	–	[59]
3,7-Dimethyl-1,6-octadien-3-yl acetate (Linalyl acetate)	196.3	0.902 (23)	HO	D_s	23	2.0e−12	–	–	[125]
Phenyl benzoate (PB)	198.2	–	AT	$D_{c\to 0}$	40–60	2.7e−9[40	5.447	84.0	[138]
Tetradecane (Alcane C_{14})	198.4	0.900 (23)	CO	D_s	23	8.2e−11	–	–	[61]
Tetradecane (Alcane C_{14})	198.4	0.902 (23)	HO	D_s	23	4.3e−11	–	–	[61]
Phenothiazine	199.3	–	IT	D	70–110	1.08e−8[70	12.01	131.2	[140]
4-Hydroxyundecanelactone acid	200.4	0.900 (23)	CO	D_s	23	1.1e−11	–	–	[54]
4-Hydroxyundecanelactone acid	200.4	0.902 (23)	HO	D_s	23	6.2e−12	–	–	[54]
4-Hydroxyundecanelactone acid	200.4	0.900 (23)	CO	D_s	23	7.0e−12	–	–	[54]
Dimethyl-3,3′-thiodipropionate	206.3	–	16.0	D	20–40	1.41e−9	5.255	79.93	[81]
Dimethyl-3,3′-thiodipropionate	206.3	–	63.0 (iT)	D	80–110	3.5e−9[70	2.447	71.56	[141]
2,6-di-*tert*-butyl-4-phenylphenol	206.3	–	–	D	140	3.24e−7[**	–	–	[142]
Pentadecane	212.3	–	37.0	D	40	2,04e−9[**	–	–	[60]
2,4-Dihydroxybenzophenone	214.2	0.898 (25)	56.0 (iT)	D	50–75	7.8e−12[40	12.64	142.3	[66]
2,4-Dihydroxybenzophenone	214.2	0.898 (25)	56.0 (iT)	D_s	44	5.5e−11[**	–	–	[66]
Dibenzyl sulphide (DBS)	214.3	–	AT	$D_{c\to 0}$	40–60	2.5e−9[40	4.748	80.0	[138]
Methyl laureate	214.4	–	64.0 (HO)	D	50–100	7.0e−12[40	11.27	134.3	[139]
Methyl laureate	214.4	–	64.0 (HO)	D	50–100	6.8e−12[40	11.45	135.5	[139]
2,5-di-*tert*-butyl-4-hydroxytoluene	220.3	–	IT	D	60–110	1.15e−9[50	6.312	94.31	[140]

Table AI.3 *(Continued)*

Diffusing Species		Polymer		Experiment		Diffusion parameters			References
Name	Molecular weight M_w (g/mol)	Density (°C) ρ_P (g/cm^3)	Crystallinity & type (%)	Type of diffusion coefficient (–)	Temperature range of experiment (°C)	Diffusion coefficient @ (23°C) D (cm^2/s)	Pre-exponential coefficient l_gD_0 (–)	Activation energy E_D (kJ/mol)	
2,6-di-*tert*-butyl-*p*-cresol (BHT)	220.3	–	54.0	D	70–100	1.16e−9(70	7.631	108.8	[143]
2,6-di-*tert*-butyl-*p*-cresol (BHT)	220.3	–	–	D	80–120	4.46e−9(70	7.503	104.1	[144]
2,6-di-*tert*-butyl-4-methylphenol (BHT)	220.3	–	–	D	25	5.0e−11(**	–	–	[67]
2,6-di-*tert*-butyl-4-methylphenol (BHT)	220.3	–	–	D_s	30–60	2.8e−12(*	7.096	105.7	[73]
2,4-Dihydroxybenzophenone (DHB)	222.2	–	–	D	25	5.0e−12(**	–	–	[79]
2-(2′-Hydroxy-5′-methyl-phenyl)-benzotriazole	225.2	–	IT	D	80–120	1.62e−8(70	3.583	74.67	[145]
2-(2′-Hydroxy-5′-methyl-phenyl)-benzotriazole	225.0	0.899	48.0 (iT)	D	40–120	8.3e−11(30	6.481	96.07	[146]
2-(2′-Hydroxy-5′-methyl-phenyl)-benzotriazole	225.3	0.899	48.0 (iT)	D	40–120	9.3e−11(30	6.274	94.57	[146]
2-(2′-Hydroxy-5′-methyl-phenyl)-benzotriazole (Tinuvin P)	225.3	–	37.0	D	40	1.5e−10(‘’	–	–	[60]
Hexadecane (Alcane C_{16})	226.4	0.900 (23)	CO	D_s	23	7.4e−11	–	–	[61]
Hexadecane (Alcane C_{16})	226.4	0.902 (23)	HO	D_s	23	3.7e−11	–	–	[61]
Hexadecane	226.4	–	37.0	D	40	1.33e−9(**	–	–	[60]
Hexadecane	226.4	–	IT	D	70–110	3.9e−9(70	3.839	80.42	[81]
2-Hydroxy-4-methoxybenzophenone	228.2	–	IT	D	70–85	2.32e−8(70	0.0792	50.64	[81]

2-Hydroxy-4-methoxybenzophenone	228.2	–	63.0 (iT)	D	80–110	1.68e−9$^{(70}$	2.826	76.17	[141]
2-Hydroxy-4-methoxybenzophenone	228.2	–	–	D	40–90	2.37e−11$^{(30}$	10.473	122.4	[147]
2-Hydroxy-4-methoxybenzophenone (Cyasorb UV9)	228.2	–	–	D	30–70	1.4e−11$^{(*}$	8.970	112.4	[148]
2-Hydroxy-4-methoxybenzophenone	228.2	–	–	D	120–160	5.6e−8$^{(100}$	2.011	66.11	[149]
2-Hydroxy-4-methoxybenzophenone	228.2	–	IT	D	60–120	2.83e−9$^{(50}$	3.980	77.45	[145]
Ethyl laureate	228.4	–	–	D	20	1.4e−11$^{(**}$	–	–	[150]
2-(2′-Hydroxy-5′-ethylphenyl)-benzotriazole	239.3	–	IT	D	80–120	1.99e−9$^{(70}$	3.915	82.83	[145]
Heptadecane	240.4	–	37.0	D	40	1.33e−9$^{(**}$	–	–	[60]
2-Hydroxy-4-ethyl-benzophenone	242.3	–	IT	D	60–120	2.82e−9$^{(50}$	3.343	73.54	[145]
Methyl miristate	242.4	–	64.0 (HO)	D	50–100	3.8e−12$^{(40}$	12.17	141.3	[139]
Methyl miristate	242.4	–	64.0 (HO)	D	50–100	4.04e−12$^{(40}$	12.02	140.3	[139]
Triphenylmethane	244.3	–	37.0	D	40	1.29e−10$^{(**}$	–	–	[60]
2,6-di-*tert*-butyl-4-i-propylphenol	247.4	–	–	D	140	3.17e−7$^{(**}$	–	–	[142]
n-Octadecane (Alcane C_{18})	254.5	0.900 (23)	CO	D_s	23	6.6e−11	–	–	[61]
n-Octadecane (Alcane C_{18})	254.5	0.902 (23)	HO	D_s	23	3.4e−11	–	–	[61]
Octadecane	254.5	–	37.0	D	40	8.67e−10$^{(**}$	–	–	[60]
n-Octadecane	254.5	–	–	D_s	30–60	1.2e−10$^{(*}$	−3.084	38.78	[77]
n-Ocatdecane	254.5	–	–	D_s	30–60	8.6e−12$^{(*}$	10.429	121.8	[73]
2-(2′-Hydroxy-5′-*n*-butylphenyl)-benzotriazole	267.3	–	IT	D	80–120	1.99e−9$^{(70}$	3.915	82.83	[145]
2-(2′-Hydroxy-5′-*t*-butyl-phenyl)-benzotriazole	267.3	–	IT	D	80–120	4.28e−9$^{(70}$	4.209	82.58	[145]
2-(2′-Hydroxy-5′-*t*-butyl-phenyl)-benzotriazole	267.3	0.899	48.0 (iT)	D	80	1.35e−8$^{(**}$	–	–	[146]
Tetramethylpentadecane	268.4	–	37.0	D	40	2.78e−10$^{(**}$	–	–	[60]
2-Hydroxy-4-*n*-butoxybenzophenone	270.3	–	24.0 (SB)	D	70–85	1.21e−8$^{(70}$	1.580	62.36	[81]
2-Hydroxy-4-*n*-butoxybenzophenone	270.3	–	63.0 (iT)	D	80–110	1.04e−9$^{(70}$	3.447	81.61	[141]

Table AI.3 *(Continued)*

Diffusing Species		Polymer		Experiment		Diffusion parameters			References
Name	Molecular weight M_w (g/mol)	Density (°C) ρ_P (g/cm^3)	Crystallinity & type (%)	Type of diffusion coefficient (–)	Temperature range of experiment (°C)	Diffusion coefficient @ (23°C) D (cm^2/s)	Pre-exponential coefficient l_gD_0 (–)	Activation energy E_D (kJ/mol)	
2-Hydroxy-4-*n*-butyl-benzophenone	270.3	–	IT	D	60–120	4.0e−10$^{(50}$	5.363	91.26	[145]
Methyl palmitate	270.4	–	64.0 (HO)	D	50–100	1.94e−12$^{(40}$	12.02	142.2	[139]
Methyl palmitate	270.4	–	64.0 (HO)	D	50–100	2.8e−12$^{(40}$	12.38	143.3	[139]
Octadecanol (Stearyl alcohol)	270.5	–	–	D	40	2.11e−10$^{(**}$	–	–	[60]
Dibuthyl phthalate (DBP)	278.3	–	–	D	20	5.1e−11$^{(**}$	–	–	[82]
Eicosane (Alcane C_{20})	282.6	0.900 (23)	CO	D_s	23	6.1e−11	–	–	[61]
Eicosane (Alcane C_{20})	282.6	0.902 (23)	HO	D_s	23	3.1e−11	–	–	[61]
N,*N*-bis(2-hydroxyphenyl)lauramide	288.0	–	–	D	40–70	6.1e−14$^{(*}$	5.962	108.7	[63]
1-Amnio-2-pentyl-antraquinone (Dye I)	293.3	–	IT	D	60–70	3.2e−10$^{(50}$	27.73	230.2	[151]
1-Amnio-2-pentyl-antraquinone (Dye I)	293.3	–	IT	D	70–90	9.3e−8$^{(70}$	15.28	146.5	[151]
2-(2′-Hydroxy-5′-cyclohexyl-phenyl)-benzotriazole	293.4	–	–	D	80–120	5.48e−10$^{(70}$	4.674	91.50	[145]
Methyl oleate	296.5	–	64.0 (HO)	D	70–90	4.0e−11$^{(60}$	11.19	137.6	[139]
Methyl oleate	296.5	–	65.9 (HO)	D	70–90	3.75e−11$^{(60}$	10.494	133.4	[139]
Methyl oleate	296.5	–	68.0 (HO)	D	70–90	4.9e−11$^{(60}$	7.711	114.8	[139]
Methyl oleate	296.5	–	70.1 (HO)	D	70–90	2.76e−11$^{(60}$	10.321	133.1	[139]
Methyl stearate	298.3	–	64.0 (HO)	D	50–110	1.3e−12$^{(40}$	12.180	144.2	[139]
Methyl stearate	298.3	–	64.0 (HO)	D	50–110	1.78e−12$^{(40}$	12.79	147.0	[139]

1-*N*-methylamino-2-pentyl-anthraquinone (Dye II)	307.4	–	IT	*D*	65–90	7.07e−8[70]	9.8	111.3	[151]
1-*N*-methylamino-2-pentyl-anthraquinone (Dye II)	307.4	–	IT	*D*	90–110	6.05e−7[100]	4.018	71.14	[151]
2,6-di-*tert*-butyl-4-(1-phenylethyl)phenol	310.5	–	–	*D*	140	3.89e−8[**]	–	–	[142]
Docosane (Alcane C_{22})	310.6	0.900 (23)	CO	D_s	23	2.9e−11	–	–	[61]
Docosane (Alcane C_{22})	310.6	0.902 (23)	HO	D_s	23	2.6e−11	–	–	[61]
Docosane	310.6	–	37.0	*D*	40	2.45e−10[**]	–	–	[60]
2-(2′-Hydroxy-5′-(1′′-phenylethyl)-phenyl) benzotriazole	315.4	–	IT	*D*	80–120	1.0e−10[70]	5.123	99.24	[145]
1-(3′-Methyl-4′-hydroxy)phenyl-4-phenyl-disazobenzene (Yellow 7)	316.5	–	IT	*D*	92–115	1.60e−7[100]	11.96	133.9	[151]
Heptadecylbenzene (Squalane)	316.6	–	37.0	*D*	40	5.24e−10[**]	–	–	[60]
2-(2′-Hydroxy-3′-*t*-butyl-5′-methyl-phenyl)-5-benzotriazole	316.6	0.899	48.0 (iT)	*D*	80	5.37e−10[**]	–	–	[146]
2,6-di-*tert*-butyl-4-*n*-octylphenol	318.5	–	–	*D*	140	1.95e−8[**]	–	–	[142]
2-(2′-Hydroxy-5′-(1′′,1′′,3′′, 3′′-tetramethyl-butyl)-phenyl)-benzotriazole	323.4	0.899	48.0 (iT)	*D*	80	3.19e−10[**]	–	–	[146]
2-(2′-Hydroxy-3′-*t*-butyl-5′-(1′′-methyl-propyl)-phenyl)-benzotriazole	323.4	0.899	48.0 (iT)	*D*	80	6.13e−10[**]	–	–	[146]
2-(2′-Hydroxy-3′,5′-di-*t*-butyl-phenyl)-benzotriazole	323.4	0.899	48.0 (iT)	*D*	60–80	3.1e−10[60]	9.722	122.5	[146]
2-(2′-Hydroxy-3′,5′-di-*t*-butyl-phenyl)-benzotriazole	323.4	0.899	48.0 (iT)	*D*	50–80	6.7e−11[50]	10.556	128.2	[146]
2-(2′-Hydroxy-3′,5′-di-*t*-butyl phenyl)-5-chlorobenzotriazole	323.4	–	IT	*D*	80–120	1.46e−10[70]	7.322	112.64	[145]

Table AI.3 *(Continued)*

Diffusing Species		Polymer		Experiment		Diffusion parameters			References
Name	Molecular weight M_w (g/mol)	Density (°C) ρ_P (g/cm^3)	Crystallinity & type (%)	Type of diffusion coefficient (–)	Temperature range of experiment (°C)	Diffusion coefficient @ (23°C) D (cm^2/s)	Pre-exponential coefficient l_gD_0 (–)	Activation energy E_D (kJ/mol)	
2-(2′-Hydroxy-5′-*n*-octyl phenyl)-benzotriazole	324.4	–	IT	*D*	80–120	7.9e−11(70	6.107	106.43	[145]
2-(2′-Hydroxy-5′-*t*-octyl phenyl)-benzotriazole	324.4	–	IT	*D*	80–120	7.9e−11(70	3.769	84.53	[145]
2,6-di-*tert*-butyl-4-dimethylbenzylphenol	324.5	–	–	*D*	140	3.58e−8(**	–	–	[142]
2-Hydroxy-4-*n*-octoxybenzophenone	326.4	–	24.0 (SB)	*D*	70–85	1.34e−8(70	2.771	69.89	[81]
2-Hydroxy-4-octoxybenzophenone	326.4	0.898	56.0 (iT)	*D*	44–75	9.1e−11(40	5.648	93.99	[84]
2-Hydroxy-4-*n*-octoxybenzophenone	326.4	–	63.0 (iT)	*D*	80–110	5.5e−10(70	4.000	87.05	[141]
2-Hydroxy-4-octoxybenzophenone (HOB)	326.4	–	–	*D*	25	1.5e−11(**	–	–	[67]
2-Hydroxy-4-*n*-octyl-benzophenone	326.4	–	IT	*D*	60–120	4.5e−12(50	8.135	120.5	[145]
2-Hydroxy-4-*n*-octyl-benzophenone	326.4	–	IT	*D*	60–120	7.9e−12(50	8.499	121.2	[145]
2-Hydroxy-4-octoxybenzophenone	326.5	–	–	*D*	30–125	1.97e−11(*	6.377	96.80	[147]
2-Hydroxy-4-octoxybenzophenone	326.5	–	35.4	*D*	75–90	3.55e−9(70	9.81	119.9	[147]
2-Hydroxy-4-octoxybenzophenone	326.5	–	48.4	*D*	75–90	7.72e−9(70	9.346	115.0	[147]
2-Hydroxy-4-octoxybenzophenone (Chimassorb 81)	326.5	–	–	*D*	40	1.5e−10(‘’	–	–	[152]
4-Alkoxy-2-hydroxybenzophenone (Cyasorb UV 531)	326.5	–	58.0	*D*	60–90	3.2e−9(60	4.513	82.92	[153]

2-Hydroxy-4-octyloxybenzophenone (Cyasorb UV 531)	326.5	–	–	*D*	30–100	1.2e−12(*	6.948	107.00	[148]
Docosanol	326.6	–	–	*D*	40	2.0e−10(**	–	–	[60]
2-(2′-Hydroxy-5′-(2″-phenyl-2″-propyl)-phenyl) benzotriazole	329.5	–	IT	*D*	80–120	1.0e−10(70	5.114	99.24	[145]
Tetracosane	338.6	–	–	*D*	40	5.61e−10(**	–	–	[60]
di-*n*-hexyl-3,3′-thiodipropionate	346.5	–	24.0 (SB)	*D*	70–85	1.04e−7(70	5.255	80.35	[81]
di-*n*-hexyl-3,3′-thiodipropionate	346.5	–	63.0 (iT)	*D*	80–110	1.53e−9(70	3.041	77.84	[141]
2-(2′-Hydroxy-3′,5′-di-(1,1″dimethylpropyl)-phenyl)-benzotriazole	351.5	0.899	48.0 (iT)	*D*	80	6.21e−9(**	–	–	[146]
n-Octadecyldiethanolamine	357.6	–	60.0	$D_{c\to 0}$	78–135	2.9e−9(70	4.156	85.72	[113]
2-(2′-Hydroxy-3′,5′-di-*t*-butyl-phenyl)-5-chlorobenzotriazole	357.9	0.899	48.0 (iT)	*D*	80	3.47e−9(**	–	–	[146]
n-Amido bis(2,3,6,6-tetramethyl-4-piperidinyl)-β-amino propionamide	366.6	0.905	IT	*D*	80–90	1.2e−9(70	4.432	87.64	[87]
Tritolylester phosphoric acid (TCP)	368.4	–	–	*D*	70	2e−13(**	–	–	[82]
2-(2′-Hydroxy-5′-*n*-dodecyl phenyl)–benzotriazole	379.5	–	IT	*D*	80–120	7.4e−11(70	−0.717	61.83	[145]
2,4-Dihydroxy-*n*-dodecocxybenzophenone	382.5	–	24.0 (SB)	*D*	70–85	2.14e−8(70	5.079	83.70	[81]
2,4-Dihydroxy-*n*-dodecocxybenzophenone	382.5	–	63.0 (iT)	*D*	80–110	4.0e−10(70	4.179	89.14	[141]
2,4-Dihydroxy-dodecocxybenzophenone	382.5	–	–	*D*	40–90	6.2e−11(30	5.749	92.56	[147]
2-Hydroxy-4-dodecyloxybenzophenone (Aduvex 2412)	382.5	–	–	*D*	30–70	5.2e−12(*	9.578	118.2	[148]
2-Hydroxy-4-*n*-dodecyl-benzophenone	382.5	–	IT	*D*	100–120	3.32e−10(100	5.141	104.38	[145]

Table AI.3 *(Continued)*

Diffusing Species		Polymer		Experiment		Diffusion parameters			References
Name	Molecular weight M_w (g/mol)	Density (°C) ρ_P (g/cm^3)	Crystallinity & type (%)	Type of diffusion coefficient (–)	Temperature range of experiment (°C)	Diffusion coefficient @ (23°C) D (cm^2/s)	Pre-exponential coefficient l_gD_0 (–)	Activation energy E_D (kJ/mol)	
2-Hydroxy-4-(2′-ethylhexyl)-5-*t*-butyl-benzophenone	382.5	–	IT	*D*	80–120	3.2e−10[70]	9.683	132.47	[145]
di-(2-ethylhexyl)-phthalate (DEHP)	390.4	–	37.0	*D*	40	3.77e−11[**	–	–	[60]
Phthalic acid bis(2-ethylhexyl ester) (DOP)	390.6	–	–	*D*	40–70	1.3e−12[40	2.386	85.52	[82]
Octacosane	394.6	–	–	*D*	40	1.78e−10[**	–	–	[60]
2,2,6,6-Tetramethyl-4-piperidinol (Dastib 845)	411.2	0.899	48.0 (iT)	*D*	25–60	7.4e−13[*	14.29	149.7	[89]
2,2,6,6-Tetramethyl-4-piperidinol (Dastib 845)	411.2	0.905	IT	*D*	60–90	1.26e−9[60	8.201	109.0	[87]
Bis(4-ethylbenzylidene)sorbitol	414.0	–	–	*D*	40–100	1.5e−13[*	4.603	98.8	[63]
Heptadeylbenzene	422.5	–	37.0	*D*	40	9.9e−11[**	–	–	[60]
2,5-di(5-*tert*-butyl-2-benzoxazolyl)-thiophene (Uvitex OB)	430.5	–	–	*D*	50–125	7.12e−11[50	5.172	94.72	[147]
2,5-Bis(5-*tert*-butyl-benzoxazol-2-yl)-thiophene (Uvitex OB)	430.0	–	37.0	*D*	40	4.1e−11[**	–	–	[60]
1,1-Bis-(2-hydroxy-3,5-di-*tert*-butylphenyl)ethane (Isonox 129)	439.0	–	–	*D*	40–121	1.4e−14[*	11.426	143.3	[63]

2-(2′-Hydroxy-3′,5′-di-(dimethylbutyl)-phenyl)-benzotriazole	447.6	0.899	48.0 (iT)	D	60–120	$1.0e{-10}^{(60}$	7.112	109.1	[146]
2-(2′-Hydroxy-3′,5′-di-(dimethylbutyl)-phenyl)-benzotriazole	447.6	0.899	48.0 (iT)	D	60–120	$8.9e{-11}^{(60}$	7.698	113.1	[146]
Dotriacontane (Alcane C_{32})	450.9	–	–	D_s	60	$6.3e{-10}^{(**}$	–	–	[75]
Dotriacontane	450.9	–	–	D_s	30–60	$5.6e{-13}^{(*}$	1.524	155.83	[73]
2-Hydroxy-4-*n*-octadecocxybenzophenone	466.7	–	24.0 (SB)	D	70–85	$6.5e{-9}^{(70}$	3.415	76.17	[81]
2-Hydroxy-4-*n*-octadecocxybenzophenone	466.7	–	24.0 (SB)	D	80–110	$2.2e{-10}^{(70}$	5.491	99.18	[141]
3,5-di-*tert*-butyl-hydroxybenzoic acid, hexadecyl ester (Cyasorb UV 2908)	475.0	–	–	D	40–70	$1.5e{-13}^{(*}$	10.557	132.5	[63]
Bis[2,2,6,6-tetramethyl-4-piperidinyl)-sebacate (Tinuvin 770)	480.7	0.899	48.0 (iT)	D	40–80	$1.8e{-12}^{(*}$	–	–	[89]
Bis[2,2,6,6-tetramethyl-4-piperidinyl)-sebacate (Tinuvin 770)	480.7	0.905	IT	D	57–83	$2.2e{-10}^{(50}$	5.802	95.6	[87]
Sebaic acid, bis(2,2,6,6-tetramethyl-piperidyl)ester (Sanol LS-770)	481.0	–	–	D	60–110	$1.3e{-11}^{(50}$	3.243	87.3	[63]
1,4-di-(2′-hydroxy-4′-oxy-benzophenone)-*n*-butane	482.5	–	IT	D	60–120	$1.04e{-10}^{(50}$	6.700	103.14	[145]
3-(3′-(5″-Chloro-2″-benzotriazole)-4′-hydroxy-5′-*t*-butyl-phenyl-propionate	486.0	0.899	48.0 (iT)	D	80	$1.8e{-9}^{(**}$	–	–	[146]
2,2-Ethyldiene-bis(4,6-di-tertbutyl-phenyl) fluoro-phosphonite	487.0	–	–	D	40	$1.2e{-12}^{(**}$	–	–	[63]
Hexatriacontane	507.0	–	37.0	D	40	$2.0e{-11}^{(**}$	–	–	[152]
Bis[2,2,6,6-tetramethyl-4-piperidinyl-1-oxy]sebacate	511.0	0.899	48.0 (iT)	D	70–121	$5.2e{-10}^{(70}$	6.223	101.8	[89]

Table AI.3 *(Continued)*

Diffusing Species		Polymer		Experiment		Diffusion parameters			References
Name	Molecular weight M_w (g/mol)	Density (°C) ρ_P (g/cm^3)	Crystallinity & type (%)	Type of diffusion coefficient (–)	Temperature range of experiment (°C)	Diffusion coefficient @ (23°C) D (cm^2/s)	Pre-exponential coefficient l_gD_0 (–)	Activation energy E_D (kJ/mol)	
Didodecyl-3-3-thiodipropionate (DLTDP)	514.4	–	60.0	D	56–135	3.41e−11$^{(50}$	3.931	82.85	[113]
di-*n*-dodecyl-3-3-thiodipropionate (DLTDP)	514.4	–	63.0 (iT)	D	80–110	6.6e−10$^{(70}$	3.756	84.95	[141]
Phosphorous acid, bis(2,4-di-*tert*-butyl-6-methylphenyl)ethyl ester (Irgafos 38)	515.0	–	–	D	40–70	1.2e−13$^{(*}$	−0.054	74.0	[63]
Thiodipropionic acid	515.6	–	37.0	D	40	2.0e−11$^{(**}$	–	–	[152]
3-(3,5-di-*tert*-butyl-4-hydroxyphenyl) propionate (Irganox 1076)	531.4	0.900	60.0	D_s	49–121	1.1e−10$^{(40}$	1.908	71.0	[117]
3-(3,5-di-*tert*-butyl-4-hydroxyphenyl) propionate (Irganox 1076)	531.4	0.900	60.0	D_s	50–135	1.0e−10$^{(40}$	4.559	87.23	[116]
3-(3,5-di-*tert*-butyl-4-hydroxyphenyl) propionate (Irganox 1076)	531.4	–	37.0	D	40	7.0e−12$^{(**}$	–	–	[152]
3-(3,5-di-*tert*-butyl-4-hydroxyphenyl) propionate (Irganox 1076)	531.4	–	–	D	40	1.2e−13$^{(**}$	–	–	[63]
3-(3,5-di-*tert*-butyl-4-hydroxyphenyl) propionate (Irganox 1076)	531.4	–	–	D	23	1.3e−11$^{(**}$	–	–	[92]
Amines bis(hydrogenated tallow alkyl) oxidized mixture	537.0	–	–	D	40–100	2.2e−13$^{(*}$	5.032	100.3	[63]

1,4-di-(2′-hydroxy-4′-oxy-benzophenone)-*n*-octene	538.5	–	IT	*D*	60–100	1.95e−10(50	6.567	100.64	[145]
1-1-3-tris(2-methyl-4-hydroxy-5-*tert*-butyl-phenyl) butane	544.5	–	60.0	*D*	100–150	9.3e−10(100	5.067	100.66	[113]
Tetracontane	563.0	–	37.0	*D*	40	1.0e−11(**	–	–	[152]
1,4-di-(2′-hydroxy-5′-*t*-butyl-4′-oxy-benzophenone)-*n*-butane	594.5	–	IT	*D*	80–120	2.7e−10(70	4.740	100.48	[145]
Bis(2,4-di-*tert*-butylphenyl) pentaerythritol diphosphite (Ultranox 626)	604.0	–	–	*D*	40–100	1.3e−13(*	10.221	130.9	[63]
Bis(2,4-di-*tert*-butylphenyl) pentaerythritol diphosphite (Ultranox 626)	605.0	–	–	*D*	40	6.5e−13(**	–	–	[63]
Bis(2,6-di-*tert*-butyl-4-methylphenyl) pentaerythritol diphosphite (Mark PEP-36)	633.0	–	–	*D*	49	2.5e−12(**	–	–	[63]
Triluarin	639.0	–	37.0	*D*	40	7.0e−12(**	–	–	[152]
Phosphorous acid, tris(2,4-di-*tert*-butylphenyl) ester (Irgafos 168)	647.0	–	37.0	*D*	40	2.5e−13(**	–	–	1528
1,4-di-(2′-hydroxy-5′-*t*-butyl-4′-oxy-benzophenone)-*n*-octane	650.9	–	– (iT)	*D*	80–120	2.8e−11(70	4.960	101.88	[145]
Bis-(2-hydroxy-3 (2′-benzotriazole-5 (1″,1″,3′,3″-tetramethyl-butyl)-phenyl)-methane	658.9	0.899	48.0 (iT)	*D*	80	7.71e−10(**	–	–	[145]
1,4-di-(2′-hydroxy-5′-(1″-phenyl-ethyl)-4′-oxy-benzophenone)-*n*-butane	690.8	–	– (iT)	*D*	80–120	2.5e−11(70	9.528	132.18	[145]

Table AI.3 *(Continued)*

Diffusing Species		Polymer		Experiment		Diffusion parameters			References
Name	**Molecular weight M_w (g/mol)**	**Density (°C) ρ_P (g/cm^3)**	**Crystallinity & type (%)**	**Type of diffusion coefficient (–)**	**Temperature range of experiment (°C)**	**Diffusion coefficient @ (23°C) D (cm^2/s)**	**Pre-exponential coefficient l_gD_0 (–)**	**Activation energy E_D (kJ/mol)**	
3,9-bis(2-(3-(*tert*-butyl-4-hydroxy-5-methylphenyl) propionyloxy)-*tert*-butyl)-2,4,8, 10-tetraoxaspiro[5,5]undecane (Sumilizer GA-80)	741.0	–	–	*D*	49	4.7e−13(**	–	–	[63]
Hexanediol-di-3-(3′-(2″-benzotriazole)-4′-hydroxy-5′-*t*-butyl-phenyl)-propionate	760.9	0.899	48.0 (iT)	*D*	80	1.06e−9(**	–	–	[146]
1-3-5-(3,5-di-*tert*-butyl-4-hydroxy benzyl) mesitylene (Irganox 1330)	774.6	–	–	*D*	80–120	3.8e−11(70	7.492	117.63	[154]
1-3-5-(3,5-di-*tert*-butyl-4-hydroxy benzyl) mesitylene (Irganox 1330)	774.6	–	37.0	*D*	40	2.0e−13(‘’	–	–	[152]
Tripalmitin	807.3	–	37.0	*D*	40	3.0e−13(**	–	–	[152]

Poly(6-(*N*-(2,2,6,6-tetramethyl-4-piperidinyl)-*n*-butylamino)-1,3,5-triazine-2,4-diyl)(2,2,6,6-tertamethyl-4-piperidinyl)imono-1,6-hexanediyl((2,2,6,6-tertamethyl-4-piperidinyl)imino-α-(*N*,*N*,*N*,*N*′-tetrabutyl-*N*‴-(2,2,6,6-tertamethyl-4-piperidinyl)imino)(Chimassorb 2020)	1060	–	–	*D*	60	1.3e−11(**	–	–	[63]
Tetrakis[3-(3-5-di-*tert*-butyl-4-hydroxy-phenyl)propionyloxymethyl)-methane (Irganox 1010)	1177.8	0.900	60.0	D_s	49–121	5.4e−13(*	5.380	100.0	[117]
Tetrakis[3-(3-5-di-*tert*-butyl-4-hydroxy-phenyl)propionyloxymethyl)-methane (Irganox 1010)	1177.8	0.900	60.0	D_s	50–135	2.47e−12(40	8.609	121.1	[118]
Tetrakis[3-(3-5-di-*tert*-butyl-4-hydroxy-phenyl)propionyloxymethyl)-methane (Irganox 1010)	1177.8	–	–	D_s	49–135	1.3e−13(40	10.397	139.4	[119]
Tetrakis[3-(3-5-di-*tert*-butyl-4-hydroxy-phenyl)propionyloxymethyl)-methane (Irganox 1010)	1177.8	0.900	48.0	*D*	70–105	1.3e−11(70	11.15	144.6	[95]
Tetrakis[3-(3-5-di-*tert*-butyl-4-hydroxy-phenyl)propionyloxymethyl)-methane (Irganox 1010)	1177.8	–	–	*D*	40	2.7e−14(**	–	–	[63]

Table AI.3 *(Continued)*

Diffusing Species		Polymer		Experiment		Diffusion parameters			References
Name	Molecular weight M_w (g/mol)	Density (°C) ρ_P (g/cm^3)	Crystallinity & type (%)	Type of diffusion coefficient (–)	Temperature range of experiment (°C)	Diffusion coefficient @ (23°C) D (cm^2/s)	Pre-exponential coefficient l_gD_0 (–)	Activation energy E_D (kJ/mol)	
N',N'-bis(2,2,6,6-tertamethyl-4-piperidinyl-2,9,15,22-tetrakis (2,2,6,6-tetramethyl-4-pipiperidinyl) 2,9,11,13,15,22,24,26,27, 28-decaazatricyclo[21.3.1.1.10.14]-octacosa-1827),10,12,14(28),23, 25-hexane-12,25-dibutyldiamine	1364.0	–	–	D	60–100	6.1e−15[40]	19.10	199.7	[155]
N,N'-bis[2,4-bis[N-(2,2,6, 6-tertamethyl-4-piperidinyl) butylaminol-1,3,5-triazine-6-yl]-N, N'-bis(2,2,6,6-tetramethyl-4-pipiperidinyl)-1,6-hexanediamine	1393.0	–	–	D	60–100	3.3e−16[40]	15.52	170.2	[155]
2,2,2-Nitrilo(triethyl-tris(3,3,5, 5-tetra-*tert*-butyl-1,1-biphenyl-2, 2-diyl)phosphite (Irgafos 12)	1465.0	–	–	D	40–100	1.3e−14[*	2.055	90.3	[63]

1,3,5-Triazine-2,4,6-triamine,*N*,*N‴*-1,2-ethanediyl-bis[*N*-[3-[[4,6-bis(butyl(1,2,2,6,6-pentamethyl-4-piperininyl) amino]-1,3,5-triazine-2-2yl] methylamino] propyl]-*N′*,*N″*-dibutyl-*N′*,*N″*-bis[1,2,2,6,6-pentamethyl-4-piperidinyl)	2286.0	–	–	*D*	70–100	$1.1e{-}13^{(50}$	15.52	130.3	[155]
N^{III},N^{IV}-bis(2,2,6,6-tertamethyl-4-piperidinyl-N^{III},N^{IV}-bis[*N′*,*N′*-dibutyl-*N″*-[6-[[4-butyl-(2,2,6,6-tetramethyl-4-pipiperidinyl)-amino-6-yl-1,3,5-triazine-2-yl]-(2,2,6,6-tetramethyl-4-pipiperidinyl)-amino-hexyl]-*N*,*N′*,*N″*-tris(2,2,6,6-tetramethyl-4-pipiperidinyl)-1,3,5-triazine-2,4,6-triamine]-1,6-hexanediamine	2758.0	–	–	*D*	70–130	$1.0e{-}14^{(50}$	15.91	185.1	[155]

where D_0 – cm^2/s – is a pre-exponential factor, E_d – kJ/mol – the energy of activation, R – 8.31 J/mol grd. – the gas constant, and T – K – the absolute temperature.

In the eigth and ninth columns D_0 and E_d are summarized for the experiments in which diffusion data were collected at different temperatures. Using these parameters with the above equation allows one to calculate the diffusion coefficient at any T point within the corresponding T range given in column 6. Moreover, one can calculate by extrapolation D's even beyond such a T range. However when doing so it is recommended not to exceed the extrapolation to far from the T range in which the experimental data were collected – column 6. Extrapolations up to $+/-$ 25% of the T range given in column 6 would most likely be on the safe side. Even when doing such a conservative extrapolation one should take care that for the new T the polymer did not change from rubbery to glassy or vice versa. It is known that for most of the polymers D_0 and E_d are usually differing in these two phases.

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