Comparison of experimental and estimated polarizabilities for organic compounds using ThermoML Archive data

Axel Drefahl
E-mail: axeleratio@yahoo.com
Internet: www.axeleratio.com

We compare values for the experimentally derived and estimated molecular polarizability for compounds that have not been used in the original design of the estimation method. The compounds along with mass density, ρ, and refractive index (Na-D line), n_D, have been extracted from the ThermoML Archive (status: February, 2007).

Experimental polarizability values are those calculated with the Lorentz-Lorenz (LL) equation from observed data for the liquid density, ρ, and the refractive index (Na-D line), n_{D}:

$$\alpha_{\mathrm{LL}} = 0.3964 \, \frac{n_{\mathrm{D}}^2 - 1}{n_{\mathrm{D}}^2 + 2} \frac{M}{\rho} \tag{1}$$

Estimated polarizability values are those estimated the atom additivity (AA) approach of Bosque and Sales (*J.Chem.Inf.Comput.Sci.***2003**,*42*,1154-1163):

$$\alpha_{\mathrm{AA}} = 0.32 + \Sigma c_{\mathrm{A}} \, N_{\mathrm{A}} \tag{2}$$

where c_{A} is the contribution for atom with element symbol A and N_{A} is number of respective atoms per molecule. A can be C, H, O, S, N, P, F, Cl, Br, and I. The summation is over all element symbols

Pearson's correlation coefficient values are those estimat

$$R = \frac{\Sigma(d_{\mathrm{AA}} d_{\mathrm{LL}})}{(\Sigma d_{\mathrm{AA}}^2 \Sigma d_{\mathrm{LL}}^2)^{1/2}} \tag{3}$$

where $d_{\mathrm{AA}} = \alpha_{\mathrm{AA},i} - \bar{\alpha}_{\mathrm{AA}}$ and $d_{\mathrm{LL}} = \alpha_{\mathrm{LL},i} - \bar{\alpha}_{\mathrm{LL}}$. Each summation is done over all i pairs. The pairs $(\alpha_{\mathrm{AA}}, \alpha_{\mathrm{LL}})$ are listed in the following for 20 and 25 °C ordered by molecular formula. The result: $R = 0.9994$ for the data at 20 °C and $R = 0.9996$ for the data 25 °C.

Compounds with experimental polarizabilities at 20 °C:

C2H2Br4
1,1,2,2-tetrabromoethane [79-27-6]
`jct/2006v38/i01/j.jct.2005.03.027`
$\alpha_{AA} = 16.85$, $\alpha_{LL} = 16.56$

C2H2Br4
1,1,2,2-tetrabromoethane [79-27-6]
`jct/2006v38/i09/2006alhalb0`
$\alpha_{AA} = 16.85$, $\alpha_{LL} = 16.56$

C2H2Cl4
1,1,1,2-tetrachloroethane [25322-20-7]
`fpe/2006v249/i01/j.fluid.2006.08.018`
$\alpha_{AA} = 12.33$, $\alpha_{LL} = 12.18$

C2H3Cl3
trichloroethane [25323-89-1]
`fpe/2006v249/i01/j.fluid.2006.08.018`
$\alpha_{AA} = 10.34$, $\alpha_{LL} = 10.23$

C3H5Cl
3-chloro-1-propene [107-05-1]
`jced/2003v48/i04/je034018b`
$\alpha_{AA} = 7.88$, $\alpha_{LL} = 8.11$

C5H10O
2-ethoxypropene [926-66-9]
`jct/2006v38/i07/j.jct.2005.10.001`
$\alpha_{AA} = 10.18$, $\alpha_{LL} = 10.53$

C5H10O
3-methyl-2-butanone [563-80-4]
`jced/2006v51/i05/je060025z.xml`
$\alpha_{AA} = 10.18$, $\alpha_{LL} = 10.02$

C5H10O2
tetrahydrofurfuryl alcohol [97-99-4]
`jced/2005v50/i02/je049605r`
$\alpha_{AA} = 10.75$, $\alpha_{LL} = 10.36$

C5H12O
2-methyl-1-butanol [137-32-6]
`jced/2004v49/i06/je030216r`
$\alpha_{AA} = 10.53$, $\alpha_{LL} = 10.57$

C6H10O4
dimethyl succinate [106-65-0]
jct/2007v39/i02/j.jct.2006.07.002
$\alpha_{AA} = 13.40$, $\alpha_{LL} = 13.09$

C6H12O2
ethyl butanoate [105-54-4]
fpe/2005v234/i01/j.fluid.2005.05.018
$\alpha_{AA} = 12.61$, $\alpha_{LL} = 12.41$

C7H12O4
dimethyl glutarate [1119-40-0]
jct/2007v39/i02/j.jct.2006.07.002.xml
$\alpha_{AA} = 15.26$, $\alpha_{LL} = 14.91$

C7H14O
5-methyl-2-hexanone [110-12-3]
fpe/2006v250/i01/j.fluid.2006.10.004
$\alpha_{AA} = 13.89$, $\alpha_{LL} = 12.57$

C7H16O3
ethyl orthoformate [122-51-0]
jct/2004v36/i11/j.jct.2004.07.023
$\alpha_{AA} = 15.38$, $\alpha_{LL} = 15.71$

C8H14O2
cyclohexyl acetate [622-45-7]
jced/2006v51/i05/je060025z
$\alpha_{AA} = 15.98$, $\alpha_{LL} = 15.40$

C8H14O2
cyclohexyl acetate [622-45-7]
jct/2005v37/i02/j.jct.2004.09.002
$\alpha_{AA} = 15.98$, $\alpha_{LL} = 15.41$

C8H14O2
cyclohexyl acetate [622-45-7]
jced/2005v50/i02/je049605r
$\alpha_{AA} = 15.98$, $\alpha_{LL} = 15.34$

C8H14O4
dimethyl adipate [627-93-0]
jct/2007v39/i02/j.jct.2006.07.002
$\alpha_{AA} = 17.12$, $\alpha_{LL} = 16.74$

C8H14O4
dimethyl adipate [627-93-0]
fpe/2005v230/i01/2005inc0
$\alpha_{AA} = 17.12$, $\alpha_{LL} = 16.51$

C8H16O
6-methyl-3-heptanone [624-42-0]
fpe/2006v250/i01/j.fluid.2006.10.004
$\alpha_{AA} = 15.75$, $\alpha_{LL} = 15.61$

C9H12
propylbenzene [103-65-1]
jced/2006v51/i01/je0502546
$\alpha_{AA} = 16.00$, $\alpha_{LL} = 16.00$

C9H20O
1-nonanol [143-08-8]
jced/2006v51/i05/je060025z
$\alpha_{AA} = 17.96$, $\alpha_{LL} = 17.93$

C10H14
butylbenzene [104-51-8]
jced/2006v51/i01/je0502546
$\alpha_{AA} = 17.85$, $\alpha_{LL} = 17.84$

C12H14O4
diethyl phthalate [84-66-2]
jct/2006v38/i11/2006xuliu0
$\alpha_{AA} = 23.16$, $\alpha_{LL} = 23.23$

C12H14O4
diethyl phthalate [84-66-2]
jct/2005v37/i10/j.jct.2005.02.005
$\alpha_{AA} = 23.16$, $\alpha_{LL} = 23.20$

C10H16
.alpha.-pinene [80-56-8]
jced/2003v48/i05/je025631i
$\alpha_{AA} = 18.20$, $\alpha_{LL} = 17.42$

C10H16
.alpha.-pinene [80-56-8]
jct/2005v37/i03/j.jct.2004.08.012
$\alpha_{AA} = 18.20$, $\alpha_{LL} = 17.42$

C18H36O

(Z)-9-octadecen-1-ol [143-28-2]
jced/2006v51/i05/je060025z
$\alpha_{AA} = 34.33$, $\alpha_{LL} = 34.34$

C18H36O
(Z)-9-octadecen-1-ol [143-28-2]
fpe/2006v250/i01/j.fluid.2006.10.005
$\alpha_{AA} = 34.33$, $\alpha_{LL} = 34.37$

C24H51N
trioctylamine [1116-76-3]
jced/2006v51/i05/je060025z
$\alpha_{AA} = 46.46$, $\alpha_{LL} = 46.52$

C28H46O4
1,2-benzenedicarboxylic acid, diisodecyl ester [26761-40-0]
jced/2005v50/i06/je050151n.xml
$\alpha_{AA} = 52.89$, $\alpha_{LL} = 52.47$

Compounds with experimental polarizabilities at 25 °C:

C4H9Cl
2-chlorobutane [78-86-4]
jct/2007v39/i01/j.jct.2006.05.003
$\alpha_{AA} = 10.08$, $\alpha_{LL} = 10.12$

C4H9Cl
isobutyl chloride [513-36-0]
jct/2007v39/i01/j.jct.2006.05.003
$\alpha_{AA} = 10.08$, $\alpha_{LL} = 10.10$

C4H9Cl
tert-butyl chloride [507-20-0]
jct/2007v39/i01/j.jct.2006.05.003
$\alpha_{AA} = 10.08$, $\alpha_{LL} = 10.21$

C4H12N2O
2-((2-aminoethyl)amino)ethanol [51251-98-0]
jced/2006v51/i04/je060032n
$\alpha_{AA} = 11.08$, $\alpha_{LL} = 11.53$

C5H8O2
vinyl propionate [105-38-4]
jced/2005v50/i02/je049909d.xml
$\alpha_{AA} = 10.40$, $\alpha_{LL} = 10.61$

C5H10Cl2
1,5-dichloropentane [628-76-2]
jct/2005v37/i12/j.jct.2005.03.020
$\alpha_{AA} = 13.93$, $\alpha_{LL} = 13.82$

C5H10O
3-methyl-2-butanone [563-80-4]
jced/2005v50/i04/je050062a
$\alpha_{AA} = 10.18$, $\alpha_{LL} = 10.04$

C5H10O2
butyl formate [592-84-7]
jct/2006v38/i09/2006ortmar0
$\alpha_{AA} = 10.75$, $\alpha_{LL} = 10.73$

C5H10O3
ethyl lactate [687-47-8]
jced/2006v51/i04/je060052p
$\alpha_{AA} = 11.32$, $\alpha_{LL} = 11.30$

C5H12O
2-methyl-1-butanol [137-32-6]
jced/2006v51/i05/je060238o
$\alpha_{AA} = 10.53$, $\alpha_{LL} = 10.60$

C5H12O
2-methyl-1-butanol [137-32-6]
jced/2005v50/i05/je0500330
$\alpha_{AA} = 10.53$, $\alpha_{LL} = 10.60$

C5H12O
2-methyl-1-butanol [137-32-6]
jced/2006v51/i02/je050420+
$\alpha_{AA} = 10.53$, $\alpha_{LL} = 10.60$

C5H12O
2-methyl-1-butanol [137-32-6]
jced/2006v51/i01/je0502142
$\alpha_{AA} = 10.53$, $\alpha_{LL} = 10.60$

C5H12O
3-methyl-2-butanol [598-75-4]
jced/2005v50/i04/je050062a
$\alpha_{AA} = 10.53$, $\alpha_{LL} = 10.57$

C5H12O2
2,2-dimethoxypropane [77-76-9]
jced/2005v50/i06/je050013y
$\alpha_{AA} = 11.10$, $\alpha_{LL} = 11.33$

C6H5Cl2OP
phenylphosphonic dichloride [824-72-6]
jced/2004v49/i03/je034263v
$\alpha_{AA} = 17.62$, $\alpha_{LL} = 17.87$

C6H5F
fluorobenzene [462-06-6]
tca/2005v439/i01/j.tca.2005.08.034
$\alpha_{AA} = 10.47$, $\alpha_{LL} = 10.30$

C6H10O4
diethyl oxalate [95-92-1]
jced/2003v48/i06/je0301489
$\alpha_{AA} = 13.40$, $\alpha_{LL} = 13.33$

C6H10O4
diethyl oxalate [95-92-1]
jced/2005v50/i03/je049610v
$\alpha_{AA} = 13.40$, $\alpha_{LL} = 13.34$

C6H12Cl2
1,6-dichlorohexane [2163-00-0]
jct/2005v37/i12/j.jct.2005.03.020
$\alpha_{AA} = 15.79$, $\alpha_{LL} = 15.69$

C6H12O2
ethyl butanoate [105-54-4]
jct/2005v37/i12/j.jct.2005.03.020
$\alpha_{AA} = 12.61$, $\alpha_{LL} = 12.48$

C6H12O2
propyl propanoate [106-36-5]
jced/2006v51/i01/je0504111
$\alpha_{AA} = 12.61$, $\alpha_{LL} = 12.48$

C6H12O2
isobutyl ethanoate [110-19-0]
fpe/2005v232/i01/2005munmon0
$\alpha_{AA} = 12.61$, $\alpha_{LL} = 12.53$

C6H12O2

tert-butyl ethanoate [540-88-5]
fpe/2005v227/i01/2005monmun0
$\alpha_{AA} = 12.61$, $\alpha_{LL} = 12.51$

C6H12O3
paraldehyde [123-63-7]
jced/2006v51/i01/je050183a
$\alpha_{AA} = 13.18$, $\alpha_{LL} = 12.93$

C6H13Cl
1-chlorohexane [544-10-5]
jct/2006v38/i07/j.jct.2005.09.003
$\alpha_{AA} = 13.80$, $\alpha_{LL} = 13.77$

C6H13Cl
1-chlorohexane [544-10-5]
tca/2005v426/i01/2005oswgar0
$\alpha_{AA} = 13.80$, $\alpha_{LL} = 13.84$

C6H14
2-methylpentane [107-83-5]
jced/2005v50/i04/je050062a
$\alpha_{AA} = 11.81$, $\alpha_{LL} = 11.88$

C6H14O2
3,6-dioxaoctane [629-14-1]
tca/2006v447/i02/2006fracom0
$\alpha_{AA} = 12.96$, $\alpha_{LL} = 13.29$

C7H12O4
dimethyl glutarate [1119-40-0]
jced/2005v50/i05/je049571n
$\alpha_{AA} = 15.26$, $\alpha_{LL} = 14.90$

C7H14O2
butyl propanoate [590-01-2]
jced/2006v51/i06/je060314n
$\alpha_{AA} = 14.47$, $\alpha_{LL} = 14.34$

C7H14O2
butyl propanoate [590-01-2]
fpe/2005v238/i01/j.fluid.2005.09.015
$\alpha_{AA} = 14.47$, $\alpha_{LL} = 14.34$

C7H14O2
butyl propanoate [590-01-2]

jct/2006v38/i09/2006ortmar0
$\alpha_{AA} = 14.47$, $\alpha_{LL} = 14.33$

C7H14O2
ethyl pentanoate [539-82-2]
jct/2005v37/i12/j.jct.2005.03.020
$\alpha_{AA} = 14.47$, $\alpha_{LL} = 14.33$

C7H14O2
ethyl isovalerate [108-64-5]
jced/2006v51/i05/je060139a
$\alpha_{AA} = 14.47$, $\alpha_{LL} = 14.36$

C7H14O2
ethyl isovalerate [108-64-5]
jced/2005v50/i05/je050170x
$\alpha_{AA} = 14.47$, $\alpha_{LL} = 14.36$

C7H16O
butane, 2-ethoxy-2-methyl- [919-94-8]
fpe/2005v233/i01/j.fluid.2005.04.003
$\alpha_{AA} = 14.24$, $\alpha_{LL} = 14.31$

C7H16O
butane, 2-ethoxy-2-methyl- [919-94-8]
jced/2004v49/i03/je0302147
$\alpha_{AA} = 14.24$, $\alpha_{LL} = 14.31$

C8H8O2
methyl benzoate [93-58-3]
jced/2006v51/i05/je060139a
$\alpha_{AA} = 14.93$, $\alpha_{LL} = 15.01$

C8H8O2
methyl benzoate [93-58-3]
jced/2005v50/i05/je050170x
$\alpha_{AA} = 14.93$, $\alpha_{LL} = 15.01$

C8H11N
DL-1-phenylethylamine [618-36-0]
jced/2005v50/i01/je0499059
$\alpha_{AA} = 15.34$, $\alpha_{LL} = 15.49$

C8H16O2
methyl heptanoate [106-73-0]
jct/2007v39/i02/j.jct.2006.07.013

$\alpha_{AA} = 16.32$, $\alpha_{LL} = 16.15$

C8H16O2
ethyl caproate [123-66-0]
jced/2005v50/i05/je050170x
$\alpha_{AA} = 16.32$, $\alpha_{LL} = 16.18$

C8H16O2
ethyl caproate [123-66-0]
jced/2006v51/i05/je0601208
$\alpha_{AA} = 16.32$, $\alpha_{LL} = 16.18$

C8H16O2
butyl butanoate [109-21-7]
jct/2006v38/i09/2006ortmar0
$\alpha_{AA} = 16.32$, $\alpha_{LL} = 16.17$

C8H18O
butyl tert-butyl ether [1000-63-1]
tca/2005v435/i02/2005arcarc0
$\alpha_{AA} = 16.10$, $\alpha_{LL} = 16.22$

C8H18O4
triglyme [112-49-2]
jced/2004v49/i02/je0302304
$\alpha_{AA} = 17.81$, $\alpha_{LL} = 18.28$

C9H10O2
benzyl acetate [140-11-4]
jced/2006v51/i05/je060139a
$\alpha_{AA} = 16.79$, $\alpha_{LL} = 16.66$

C9H10O2
benzyl acetate [140-11-4]
jced/2005v50/i05/je050170x
$\alpha_{AA} = 16.79$, $\alpha_{LL} = 16.66$

C9H18O2
isopentyl butanoate [106-27-4]
jced/2005v50/i05/je050170x
$\alpha_{AA} = 18.18$, $\alpha_{LL} = 18.03$

C9H18O2
isopentyl butanoate [106-27-4]
jced/2006v51/i05/je0601208
$\alpha_{AA} = 18.18$, $\alpha_{LL} = 18.03$

C10H12O2
benzyl propanoate [122-63-4]
jced/2006v51/i05/je060139a
$\alpha_{AA} = 18.65$, $\alpha_{LL} = 18.47$

C10H12O2
benzyl propanoate [122-63-4]
jced/2005v50/i05/je050170x
$\alpha_{AA} = 18.65$, $\alpha_{LL} = 18.47$

C10H12O2
ethyl phenylethanoate [101-97-3]
jced/2005v50/i05/je050170x
$\alpha_{AA} = 18.65$, $\alpha_{LL} = 18.49$

C10H12O2
ethyl phenylethanoate [101-97-3]
jced/2006v51/i05/je0601208
$\alpha_{AA} = 18.65$, $\alpha_{LL} = 18.49$

C10H14
butylbenzene [104-51-8]
jct/2005v37/i09/j.jct.2005.01.007
$\alpha_{AA} = 17.85$, $\alpha_{LL} = 17.88$

C10H18
trans-decalin [493-02-7]
fpe/2006v243/i01/j.fluid.2006.01.024
$\alpha_{AA} = 18.55$, $\alpha_{LL} = 17.55$

C10H18O
dl-2,6-dimethyl-2,7-octadien-6-ol [78-70-6]
fpe/2005v238/i01/j.fluid.2005.09.009
$\alpha_{AA} = 19.12$, $\alpha_{LL} = 19.50$

C10H20O2
ethyl octanoate [106-32-1]
jced/2005v50/i05/je050170x
$\alpha_{AA} = 20.04$, $\alpha_{LL} = 19.86$

C10H20O2
ethyl octanoate [106-32-1]
jced/2006v51/i05/je0601208
$\alpha_{AA} = 20.04$, $\alpha_{LL} = 19.86$

C10H22O5
dimethoxytetraglycol [143-24-8]
`jced/2004v49/i02/je0302304`
$\alpha_{AA} = 22.10$, $\alpha_{LL} = 22.63$

C12H14O4
diethyl phthalate [84-66-2]
`jced/2003v48/i06/je0301489`
$\alpha_{AA} = 23.16$, $\alpha_{LL} = 23.24$

C14H30
tetradecane [629-59-4]
`jct/2006v38/i08/2006mutman0`
$\alpha_{AA} = 26.68$, $\alpha_{LL} = 26.53$

C14H30
tetradecane [629-59-4]
`jced/2003v48/i06/je030147g`
$\alpha_{AA} = 26.68$, $\alpha_{LL} = 26.61$

C24H38O4
dioctyl phthalate [117-84-0]
`jced/2003v48/i06/je0301489`
$\alpha_{AA} = 45.45$, $\alpha_{LL} = 45.24$

C30H62
2,6,10,15,19,23-hexamethyltetracosane [111-01-3]
`ijt/2005v26/i03/2005tri0`
$\alpha_{AA} = 56.41$, $\alpha_{LL} = 55.65$

This document is supplementing the paper entitled "Extraction and Application of Environmentally Relevant Chemical Information from the ThermoML Archive" (`www.axeleratio.com/EnviroInfo2007/paper.doc`) submitted to the EnviroInfo 2007, Sept. 12-14 in Poland, Warsaw (www.enviroinfo2007.org).