Benzeneacetic acid, ethyl ester

Other names:	2-Phenylacetic acid ethyl ester
	Acetic acid, phenyl-, ethyl ester
	ETHYL ALPHA-TOLUATE
	ETHYL BENZENEACETATE
	ETHYL PHENYLETHANOATE
	Ethyl 2-phenylacetate
	Ethyl 2-phenylethanoate
	Ethyl phenacetate
	Ethyl phenylacetate
	Ethyl «alpha»-toluate
	Ethyl Â«alphaÂ»-toluate
	NSC 406259
	Phenylacetic acid, ethyl ester
	ethanoic acid, phenyl-, ethyl ester
	«alpha»-Toluic acid, ethyl ester
	Â«alphaÂ»-Toluic acid, ethyl ester
Inchi:	InChI=1S/C10H12O2/c1-2-12-10(11)8-9-6-4-3-5-7-9/h3-7H,2,8H2,1H3
InchiKey:	DULCUDSUACXJJC-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	CCOC(=O)Cc1ccccc1
Mol. weight [g/mol]:	164.20
CAS:	101-97-3

Physical Properties

Property code	Value	Unit	Source
chl	-5243.90 ± 4.20	kJ/mol	NIST Webbook
gf	-88.19	kJ/mol	Joback Method
hf	-258.00	kJ/mol	Joback Method
hfus	18.48	kJ/mol	Joback Method
hvap	64.50 ± 0.40	kJ/mol	NIST Webbook
hvap	60.70	kJ/mol	NIST Webbook
log10ws	-1.97		Crippen Method
logp	1.792		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
rinpol	1208.64		NIST Webbook
rinpol	1247.00		NIST Webbook

rinpol	1222.00	NIST Webbook
rinpol	1213.00	NIST Webbook
rinpol	1246.00	NIST Webbook
rinpol	1243.00	NIST Webbook
rinpol	1244.00	NIST Webbook
rinpol	1252.00	NIST Webbook
rinpol	1219.00	NIST Webbook
rinpol	1249.00	NIST Webbook
rinpol	1243.00	NIST Webbook
rinpol	1225.00	NIST Webbook
rinpol	1225.00	NIST Webbook
rinpol	1249.00	NIST Webbook
rinpol	1247.00	NIST Webbook
rinpol	1245.00	NIST Webbook
rinpol	1246.00	NIST Webbook
rinpol	1247.00	NIST Webbook
rinpol	1251.00	NIST Webbook
rinpol	1247.00	NIST Webbook
rinpol	1231.00	NIST Webbook
rinpol	1219.00	NIST Webbook
rinpol	1214.00	NIST Webbook
rinpol	1213.00	NIST Webbook
rinpol	1246.00	NIST Webbook
rinpol	1243.00	NIST Webbook
rinpol	1248.00	NIST Webbook
rinpol	1247.00	NIST Webbook
rinpol	1243.00	NIST Webbook
rinpol	1245.00	NIST Webbook
rinpol	1247.00	NIST Webbook
rinpol	1193.00	NIST Webbook
rinpol	1247.00	NIST Webbook
rinpol	1251.00	NIST Webbook
rinpol	1246.00	NIST Webbook
rinpol	1253.00	NIST Webbook
rinpol	1244.00	NIST Webbook
rinpol	1225.00	NIST Webbook
rinpol	1229.00	NIST Webbook
rinpol	1243.00	NIST Webbook
rinpol	1248.30	NIST Webbook
rinpol	1224.00	NIST Webbook
rinpol	1209.00	NIST Webbook
rinpol	1213.00	NIST Webbook
rinpol	1210.80	NIST Webbook
rinpol	1211.70	NIST Webbook

rinpol	1213.64	NIST Webbook
rinpol	1210.80	NIST Webbook
rinpol	1249.00	NIST Webbook
rinpol	1244.00	NIST Webbook
rinpol	1223.90	NIST Webbook
rinpol	1224.90	NIST Webbook
rinpol	1247.00	NIST Webbook
rinpol	1260.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1252.00	NIST Webbook
rinpol	1229.00	NIST Webbook
rinpol	1225.00	NIST Webbook
rinpol	1239.00	NIST Webbook
rinpol	1210.19	NIST Webbook
rinpol	1246.00	NIST Webbook
rinpol	1207.77	NIST Webbook
rinpol	1230.68	NIST Webbook
rinpol	1211.83	NIST Webbook
rinpol	1251.00	NIST Webbook
rinpol	1215.50	NIST Webbook
rinpol	1217.58	NIST Webbook
rinpol	1219.66	NIST Webbook
rinpol	1221.84	NIST Webbook
rinpol	1224.16	NIST Webbook
rinpol	1226.48	NIST Webbook
rinpol	1205.65	NIST Webbook
rinpol	1207.01	NIST Webbook
rinpol	1255.00	NIST Webbook
ripol	1755.00	NIST Webbook
ripol	1786.00	NIST Webbook
ripol	1770.00	NIST Webbook
ripol	1785.00	NIST Webbook
ripol	1782.00	NIST Webbook
ripol	1788.00	NIST Webbook
ripol	1784.70	NIST Webbook
ripol	1793.00	NIST Webbook
ripol	1754.00	NIST Webbook
ripol	1779.00	NIST Webbook
ripol	1773.00	NIST Webbook
ripol	1821.00	NIST Webbook
ripol	1797.00	NIST Webbook
ripol	1800.00	NIST Webbook
ripol	1799.00	NIST Webbook
ripol	1795.00	NIST Webbook

ripol	1790.00		NIST Webbook
ripol	1773.00		NIST Webbook
ripol	1780.00		NIST Webbook
ripol	1760.00		NIST Webbook
ripol	1785.00		NIST Webbook
ripol	1783.00		NIST Webbook
ripol	1799.00		NIST Webbook
ripol	1770.00		NIST Webbook
ripol	1823.00		NIST Webbook
ripol	1818.00		NIST Webbook
ripol	1823.00		NIST Webbook
ripol	1818.00		NIST Webbook
ripol	1785.00		NIST Webbook
ripol	1786.00		NIST Webbook
ripol	1771.00		NIST Webbook
ripol	1780.00		NIST Webbook
ripol	1775.00		NIST Webbook
ripol	1763.00		NIST Webbook
ripol	1768.00		NIST Webbook
ripol	1768.00		NIST Webbook
ripol	1770.00		NIST Webbook
ripol	1781.00		NIST Webbook
ripol	1788.00		NIST Webbook
ripol	1755.00		NIST Webbook
ripol	1767.00		NIST Webbook
ripol	1826.00		NIST Webbook
ripol	1785.00		NIST Webbook
ripol	1765.00		NIST Webbook
ripol	1786.00		NIST Webbook
ripol	1784.70		NIST Webbook
ripol	1781.80		NIST Webbook
ripol	1781.80		NIST Webbook
ripol	1778.50		NIST Webbook
ripol	1776.00		NIST Webbook
ripol	1793.00		NIST Webbook
ripol	1793.00		NIST Webbook
ripol	1775.00		NIST Webbook
ripol	1783.00		NIST Webbook
ripol	1775.00		NIST Webbook
ripol	1779.00		NIST Webbook
ripol	1782.00		NIST Webbook
tb	502.20	K	NIST Webbook
tb	500.50 ± 1.00	K	NIST Webbook
tb	501.90 ± 0.50	K	NIST Webbook

tb	501.90 ± 0.50	K	NIST Webbook
tb	500.20	K	NIST Webbook
tc	743.85	K	Joback Method
tf	301.04	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.98	J/mol×K	743.85	Joback Method
cpg	326.90	J/mol×K	602.06	Joback Method
cpg	314.07	J/mol×K	566.62	Joback Method
cpg	300.47	J/mol×K	531.17	Joback Method
cpg	361.01	J/mol×K	708.40	Joback Method
cpg	350.35	J/mol×K	672.95	Joback Method
cpg	338.99	J/mol×K	637.51	Joback Method
dvisc	0.0023840	Pa×s	298.15	Densities and Viscosities of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at T = (288.15, 298.15, 308.15, and 318.15) K
dvisc	0.0019480	Pa×s	308.15	Densities and Viscosities of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at T = (288.15, 298.15, 308.15, and 318.15) K

dvisc	0.0016240	Pa×s	318.15	Densities and Viscosities of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at T = (288.15, 298.15, 308.15, and 318.15) K
dvisc	0.0030020	Pa×s	288.15	Densities and Viscosities of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at T = (288.15, 298.15, 308.15, and 318.15) K
hvapt	54.00	kJ/mol	446.50	NIST Webbook
hvapt	63.90 ± 0.40	kJ/mol	308.00	NIST Webbook
rhol	1026.96	kg/m3	298.15	Refractive Indices and Surface Tensions of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at (288.15, 298.15, 308.15, and 318.15) K
srf	0.03	N/m	318.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K

srf	0.03	N/m	308.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.03	N/m	298.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.04	N/m	288.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.03	N/m	338.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.03	N/m	348.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.03	N/m	358.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.03	N/m	328.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.65130e+02
Coeff. B	-1.42761e+04
Coeff. C	-2.16596e+01
Coeff. D	1.00524e-05
Temperature range (K), min.	422.15
Temperature range (K), max.	506.15

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Densities and Viscosities of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at T = (288.15, 298.15, 308.15, and 318.15) K:	https://www.doi.org/10.1021/je050389b
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C101973&Units=SI
Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K:	https://www.doi.org/10.1021/je050170x
KDB Vapor Pressure Data:	https://www.cheric.org/files/research/kdb/mol/mol1145.mol
	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1145
Refractive Indices and Surface Tensions of Binary Mixtures of Isoamyl Acetate, Ethyl Caproate, Ethyl Benzoate, Isoamyl Butyrate, Ethyl Phenylacetate, and Ethyl Caprylate with Ethanol at (288.15, 298.15, 308.15, and 318.15) K:	https://www.doi.org/10.1021/je0601208
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions

hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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