Acetic acid, phenyl ester

Other names:	Fenylester kyseliny octove
	Phenol acetate
	Phenyl acetate
	Phenyl ester of acetic acid
	phenyl ethanoate
Inchi:	InChI=1S/C8H8O2/c1-7(9)10-8-5-3-2-4-6-8/h2-6H,1H3
InchiKey:	IPBVNPXQWQGGJP-UHFFFAOYSA-N
Formula:	C8H8O2
SMILES:	CC(=O)Oc1ccccc1
Mol. weight [g/mol]:	136.15
CAS:	122-79-2

Physical Properties

Property code	Value	Unit	Source
chl	-3966.00 ± 0.84	kJ/mol	NIST Webbook
gf	-105.03	kJ/mol	Joback Method
hf	-280.00 ± 2.00	kJ/mol	NIST Webbook
hf	-279.70 ± 1.20	kJ/mol	NIST Webbook
hfl	-334.80 ± 0.92	kJ/mol	NIST Webbook
hfl	-326.00 ± 0.80	kJ/mol	NIST Webbook
hfus	13.30	kJ/mol	Joback Method
hvap	53.60	kJ/mol	NIST Webbook
hvap	54.80	kJ/mol	NIST Webbook
hvap	54.00 ± 2.00	kJ/mol	NIST Webbook
hvap	55.20 ± 0.80	kJ/mol	NIST Webbook
hvap	53.10	kJ/mol	NIST Webbook
hvap	46.30	kJ/mol	NIST Webbook
hvap	53.30	kJ/mol	NIST Webbook
ie	8.75 ± 0.03	eV	NIST Webbook
ie	8.80 ± 0.20	eV	NIST Webbook
ie	8.60 ± 0.05	eV	NIST Webbook
log10ws	-1.79		Crippen Method
logp	1.612		Crippen Method
mcvol	107.260	ml/mol	McGowan Method
pc	3862.67	kPa	Joback Method
rinpol	1068.00		NIST Webbook
rinpol	1008.00		NIST Webbook

rinpol	1025.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	1025.00		NIST Webbook
rinpol	1033.00		NIST Webbook
rinpol	1033.00		NIST Webbook
rinpol	1033.00		NIST Webbook
rinpol	1050.00		NIST Webbook
rinpol	1065.00		NIST Webbook
rinpol	1068.00		NIST Webbook
ripol	1660.00		NIST Webbook
ripol	1633.00		NIST Webbook
tb	468.85 ± 0.40	K	NIST Webbook
tb	469.00 ± 4.00	K	NIST Webbook
tb	469.20	K	NIST Webbook
tb	468.00	K	NIST Webbook
tb	468.85	K	NIST Webbook
tb	469.90 ± 1.00	K	NIST Webbook
tb	468.70 ± 0.50	K	NIST Webbook
tb	468.90 ± 0.50	K	NIST Webbook
tb	468.90 ± 0.50	K	NIST Webbook
tc	705.10	K	Joback Method
tf	267.05	K	NIST Webbook
vc	0.400	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.26	J/mol×K	485.41	Joback Method
cpg	265.28	J/mol×K	668.48	Joback Method
cpg	256.31	J/mol×K	631.87	Joback Method
cpg	246.75	J/mol×K	595.25	Joback Method
cpg	236.56	J/mol×K	558.64	Joback Method
cpg	225.73	J/mol×K	522.02	Joback Method
cpg	273.64	J/mol×K	705.10	Joback Method
dvisc	0.0012822	Pa×s	312.99	Joback Method
dvisc	0.0008057	Pa×s	347.47	Joback Method
dvisc	0.0005505	Pa×s	381.95	Joback Method
dvisc	0.0004007	Pa×s	416.44	Joback Method
dvisc	0.0003062	Pa×s	450.92	Joback Method
dvisc	0.0022895	Pa×s	278.50	Joback Method
dvisc	0.0002430	Pa×s	485.41	Joback Method

hvapt	51.70	kJ/mol	390.00	NIST Webbook
pvap	66.10	kPa	453.20	Isothermal (vapour + liquid) equilibrium (VLE) for binary mixtures containing diethyl carbonate, phenyl acetate, diphenyl carbonate, or ethyl acetate
pvap	18.20	kPa	413.20	Isothermal (vapour + liquid) equilibrium (VLE) for binary mixtures containing diethyl carbonate, phenyl acetate, diphenyl carbonate, or ethyl acetate
pvap	3.50	kPa	373.20	Isothermal (vapour + liquid) equilibrium (VLE) for binary mixtures containing diethyl carbonate, phenyl acetate, diphenyl carbonate, or ethyl acetate
rhol	1073.00	kg/m3	298.20	Investigation of Ternary Phase Diagrams of (Water + Butyric Acid + Phenyl Acetate) at Different Temperatures
rhol	1073.30	kg/m3	298.15	Revision of the volumetric method for measurements of liquid liquid equilibria in binary systems

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.63860e+01

Coeff. B	-5.16870e+03
Coeff. C	-2.99210e+01
Temperature range (K), min.	350.99
Temperature range (K), max.	496.64

Sources

Isothermal (vapour + liquid) equilibrium (VLE) for binary mixtures containing diethyl carbonate, phenyl acetate, diphenyl carbonate, or ethyl acetate:	https://www.doi.org/10.1016/j.jct.2015.07.024
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Revision of the volumetric method for measurements of liquid liquid equilibria in binary systems:	https://www.doi.org/10.1016/j.fluid.2004.12.004
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C122792&Units=SI
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Investigation of Ternary Phase Diagrams of (Water + Butyric Acid + Phenyl Acetate) at Different Temperatures:	https://www.doi.org/10.1021/acs.jced.5b00950
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hfl:	Liquid phase 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
ie:	Ionization energy
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
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume