Acetic acid, 2-phenylethyl ester

Other names:	2-Phenethyl acetate
	2-Phenylethyl acetate
	Acetic acid «beta»-phenylethyl ester
	Acetic acid Â«betaÂ»-phenylethyl ester
	Acetic acid, phenethyl ester
	Benzylcarbinyl acetate
	Ethanol, 2-phenyl-, acetate
	NSC 71927
	Phenethyl acetate
	Phenethyl alcohol, acetate
	Phenylethyl acetate
	Phenylethyl acetate-«beta»
	Phenylethyl acetate-Â«betaÂ»
	phenylethyl ethanoate
	«beta»-Phenethyl acetate
	«beta»-Phenylethanol acetate
	«beta»-Phenylethyl acetate
	Â«betaÂ»-Phenethyl acetate
	Â«betaÂ»-Phenylethanol acetate
	Â«betaÂ»-Phenylethyl acetate
Inchi:	InChI=1S/C10H12O2/c1-9(11)12-8-7-10-5-3-2-4-6-10/h2-6H,7-8H2,1H3
InchiKey:	MDHYEMXUFSJLGV-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	CC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	164.20
CAS:	103-45-7

Physical Properties

Property code	Value	Unit	Source
gf	-88.19	kJ/mol	Joback Method
hf	-258.00	kJ/mol	Joback Method
hfus	18.48	kJ/mol	Joback Method
hvap	67.40	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	1250.00	NIST Webbook
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tb	505.80	K	NIST Webbook
tb	511.70	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	300.47	J/mol×K	531.17	Joback Method
cpg	314.07	J/mol×K	566.62	Joback Method
cpg	326.90	J/mol×K	602.06	Joback Method
cpg	338.99	J/mol×K	637.51	Joback Method
cpg	350.35	J/mol×K	672.95	Joback Method
cpg	361.01	J/mol×K	708.40	Joback Method
cpg	370.98	J/mol×K	743.85	Joback Method
dvisc	0.0012567	Pa×s	339.39	Joback Method
dvisc	0.0023380	Pa×s	301.04	Joback Method
dvisc	0.0007662	Pa×s	377.75	Joback Method
dvisc	0.0005118	Pa×s	416.11	Joback Method
dvisc	0.0003660	Pa×s	454.46	Joback Method
dvisc	0.0002757	Pa×s	492.81	Joback Method
dvisc	0.0002164	Pa×s	531.17	Joback Method
hvapt	61.30	kJ/mol	298.15	Vapor pressures and vaporization enthalpies of a series of esters used in flavors by correlation gas chromatography
hvapt	52.20	kJ/mol	464.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56680e+01
Coeff. B	-5.12062e+03
Coeff. C	-4.23310e+01
Temperature range (K), min.	375.26
Temperature range (K), max.	536.77

Sources

Vapor pressures and vaporization enthalpies of a series of esters used in flavors by correlation gas chromatography:	https://www.doi.org/10.1016/j.jct.2015.02.015
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103457&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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
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