Benzenemethanol, «alpha»-methyl-, acetate

Other names:	Benzyl alcohol, «alpha»-methyl-, acetate
	«alpha»-Methylbenzyl acetate
	«alpha»-Phenylethyl acetate
	sec-Phenylethyl acetate
	Gardeniol II
	Gardenol
	Methylphenylcarbinol acetate
	Methylphenylcarbinyl acetate
	Styralyl acetate
	1-Phenylethyl acetate
	Phenylmethylcarbinyl acetate
	Styrallyl acetate
	1-Acetoxy-1-phenylethane
	NSC 2397
	Styrylallyl acetate
	«alpha»-Methylbenzyl alcohol, acetate
	Acetic acid, 1-phenylethyl ester
Inchi:	InChI=1S/C10H12O2/c1-8(12-9(2)11)10-6-4-3-5-7-10/h3-8H,1-2H3
InchiKey:	QUMXDOLUJCHOAY-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	CC(=O)OC(C)c1ccccc1
Mol. weight [g/mol]:	164.20
CAS:	93-92-5

Physical Properties

Property code	Value	Unit	Source
gf	-90.63	kJ/mol	Joback Method
hf	-263.28	kJ/mol	Joback Method
hfus	14.96	kJ/mol	Joback Method
hvap	48.90	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	2.311		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
rinpol	1165.00		NIST Webbook
rinpol	1190.00		NIST Webbook
rinpol	1186.00		NIST Webbook

rinpol	1194.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1166.70		NIST Webbook
rinpol	1190.00		NIST Webbook
rinpol	1163.60		NIST Webbook
rinpol	1206.00		NIST Webbook
ripol	1673.00		NIST Webbook
ripol	1680.00		NIST Webbook
ripol	1696.00		NIST Webbook
ripol	1693.20		NIST Webbook
tb	530.73	K	Joback Method
tc	748.19	K	Joback Method
tf	286.04	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.78	J/mol×K	530.73	Joback Method
cpg	314.76	J/mol×K	566.97	Joback Method
cpg	327.92	J/mol×K	603.22	Joback Method
cpg	340.30	J/mol×K	639.46	Joback Method
cpg	351.91	J/mol×K	675.70	Joback Method
cpg	362.77	J/mol×K	711.95	Joback Method
cpg	372.90	J/mol×K	748.19	Joback Method
dvisc	0.0031130	Pa×s	286.04	Joback Method
dvisc	0.0014883	Pa×s	326.82	Joback Method
dvisc	0.0008382	Pa×s	367.60	Joback Method
dvisc	0.0005294	Pa×s	408.38	Joback Method
dvisc	0.0003634	Pa×s	449.17	Joback Method
dvisc	0.0002656	Pa×s	489.95	Joback Method
dvisc	0.0002037	Pa×s	530.73	Joback Method

Sources

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=C93925&Units=SI

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical 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