3-Phenyl-1-propanol, acetate

Other names:	Benzenepropyl acetate
	1-Propanol, 3-phenyl-, acetate
	«gamma»-Phenylpropyl acetate
	(3-Acetoxypropyl)benzene
	Hydrocinnamyl acetate
	3-Acetoxy-1-phenylpropane
	3-Phenylpropyl acetate
	Phenylpropyl acetate
	3-Phenyl-1-propyl acetate
	1-Acetoxy-3-phenylpropane
	Benzenepropanol, 1-acetate
	Benzenepropanol, acetate
	NSC 404453
	Acetic acid, 3-phenylpropyl ester
Inchi:	InChI=1S/C11H14O2/c1-10(12)13-9-5-8-11-6-3-2-4-7-11/h2-4,6-7H,5,8-9H2,1H3
InchiKey:	JRJGKUTZNBZHNK-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	CC(=O)OCCCc1ccccc1
Mol. weight [g/mol]:	178.23
CAS:	122-72-5

Physical Properties

Property code	Value	Unit	Source
gf	-79.77	kJ/mol	Joback Method
hf	-278.64	kJ/mol	Joback Method
hfus	21.07	kJ/mol	Joback Method
hvap	51.51	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.182		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
rinpol	1380.00		NIST Webbook
rinpol	1364.00		NIST Webbook
rinpol	1373.00		NIST Webbook
rinpol	1368.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1378.00		NIST Webbook

rinpol	1373.00		NIST Webbook
rinpol	1365.00		NIST Webbook
rinpol	1359.00		NIST Webbook
rinpol	1388.00		NIST Webbook
rinpol	1347.00		NIST Webbook
rinpol	1341.00		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	1365.00		NIST Webbook
rinpol	1363.00		NIST Webbook
rinpol	1363.00		NIST Webbook
rinpol	1388.00		NIST Webbook
rinpol	1382.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1357.00		NIST Webbook
rinpol	1373.00		NIST Webbook
rinpol	1380.00		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	1347.00		NIST Webbook
ripol	1917.00		NIST Webbook
ripol	1930.00		NIST Webbook
ripol	1944.00		NIST Webbook
ripol	1971.00		NIST Webbook
ripol	1930.00		NIST Webbook
ripol	1919.00		NIST Webbook
ripol	1965.00		NIST Webbook
ripol	1926.00		NIST Webbook
ripol	1936.00		NIST Webbook
ripol	1947.40		NIST Webbook
ripol	1941.00		NIST Webbook
ripol	1971.00		NIST Webbook
ripol	1917.00		NIST Webbook
tb	500.00 ± 4.00	K	NIST Webbook
tc	763.32	K	Joback Method
tf	312.31	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	410.76	J/mol×K	728.44	Joback Method
cpg	399.42	J/mol×K	693.56	Joback Method
cpg	387.33	J/mol×K	658.68	Joback Method
cpg	374.48	J/mol×K	623.81	Joback Method
cpg	360.84	J/mol×K	588.93	Joback Method
cpg	346.39	J/mol×K	554.05	Joback Method
cpg	421.37	J/mol×K	763.32	Joback Method
dvisc	0.0023060	Pa×s	312.31	Joback Method
dvisc	0.0002006	Pa×s	554.05	Joback Method
dvisc	0.0002569	Pa×s	513.76	Joback Method
dvisc	0.0003432	Pa×s	473.47	Joback Method
dvisc	0.0004838	Pa×s	433.18	Joback Method
dvisc	0.0007317	Pa×s	392.89	Joback Method
dvisc	0.0012165	Pa×s	352.60	Joback Method
hvapt	74.30	kJ/mol	313.00	NIST Webbook
hvapt	56.80	kJ/mol	454.00	NIST Webbook

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=C122725&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
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

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