Benzenepropanal

Other names:	3-Phenyl-1-propanal
	3-Phenylpropan-1-al
	3-Phenylpropanal
	3-Phenylpropionaldehyde
	3-Phenylpropylaldehyde
	Benzylacetaldehyde
	Dihydrocinnamaldehyde
	Hydrocinnamaldehyde
	Hydrocinnamic aldehyde
	NSC 9271
	Propionaidehyde, 3-phenyl-
	phenyl propionaldehyde
	«beta»-Phenylpropionaldehyde
	Â«betaÂ»-Phenylpropionaldehyde
Inchi:	InChI=1S/C9H10O/c10-8-4-7-9-5-2-1-3-6-9/h1-3,5-6,8H,4,7H2
InchiKey:	YGCZTXZTJXYWCO-UHFFFAOYSA-N
Formula:	C9H10O
SMILES:	O=CCCc1ccccc1
Mol. weight [g/mol]:	134.18
CAS:	104-53-0

Physical Properties

Property code	Value	Unit	Source
gf	37.79	kJ/mol	Joback Method
hf	-78.14	kJ/mol	Joback Method
hfus	15.40	kJ/mol	Joback Method
hvap	44.62	kJ/mol	Joback Method
log10ws	-1.97		Crippen Method
logp	1.818		Crippen Method
mcvol	115.480	ml/mol	McGowan Method
pc	3555.77	kPa	Joback Method
rinpol	1178.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1178.00		NIST Webbook

rinpol	1123.00		NIST Webbook
rinpol	1122.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1180.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1146.00		NIST Webbook
rinpol	1146.00		NIST Webbook
ripol	1745.00		NIST Webbook
ripol	1783.00		NIST Webbook
ripol	1809.00		NIST Webbook
ripol	1809.00		NIST Webbook
ripol	1793.00		NIST Webbook
ripol	1723.00		NIST Webbook
ripol	1745.00		NIST Webbook
ripol	1783.00		NIST Webbook
ripol	1761.00		NIST Webbook
ripol	1723.00		NIST Webbook
ripol	1783.00		NIST Webbook
ripol	1793.00		NIST Webbook
tb	480.66	K	Joback Method
tc	693.34	K	Joback Method
tf	259.61	K	Joback Method
vc	0.449	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.47	J/mol×K	693.34	Joback Method
cpg	234.85	J/mol×K	480.66	Joback Method
cpg	247.43	J/mol×K	516.11	Joback Method
cpg	259.25	J/mol×K	551.55	Joback Method
cpg	270.33	J/mol×K	587.00	Joback Method
cpg	280.70	J/mol×K	622.45	Joback Method

cpg	290.40	J/mol×K	657.89	Joback Method
dvisc	0.0002938	Pa×s	480.66	Joback Method
dvisc	0.0034100	Pa×s	259.61	Joback Method
dvisc	0.0017581	Pa×s	296.45	Joback Method
dvisc	0.0010494	Pa×s	333.29	Joback Method
dvisc	0.0006941	Pa×s	370.13	Joback Method
dvisc	0.0004948	Pa×s	406.98	Joback Method
dvisc	0.0003731	Pa×s	443.82	Joback Method
hvapt	67.50	kJ/mol	346.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	370.70	K	1.60	NIST Webbook
tbrp	377.70	K	1.70	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104530&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Quantitative NMR spectroscopy of binary liquid mixtures (aldehyde + alcohol). Part III: (1-decanal or 3-phenylpropanal or 2-chlorobenzaldehyde) + (methanol or ethanol or 1-propanol):	https://www.doi.org/10.1016/j.jct.2014.01.027
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume