2-Propenal, 3-phenyl-

Other names:	(E)-3-phenyl-2-propanal
	2-Propenaldehyde, 3-phenyl-
	3-Fenylpropenal
	3-Phenyl-2-propen-1-al
	3-Phenyl-2-propenal (cinnamaldehyde)
	3-Phenylacrylaldehyde
	3-phenyl-2-propenal
	3-phenyl-2-propenaldehyde
	3-phenylacrolein
	3-phenylpropenal
	Abion CA
	Acrolein, 3-phenyl-
	Aldehyd skoricovy
	Benzylideneacetaldehyde
	Cinnamylaldehyde
	NCI-C56111
	NSC 16935
	Propenaldehyde, 3-phenyl-
	Zimtaldehyde
	cassia aldehyde
	cinnamal
	cinnamaldehyde
	cinnamaldehyde (3-phenyl-2-propenal)
	cinnamic aldehyde
	cinnamyl aldehyde
	phenylacrolein
	trans-3-phenyl-2-propenal
Inchi:	InChI=1S/C9H8O/c10-8-4-7-9-5-2-1-3-6-9/h1-8H
InchiKey:	KJPRLNWUNMBNBZ-UHFFFAOYSA-N
Formula:	C9H8O
SMILES:	O=CC=Cc1ccccc1
Mol. weight [g/mol]:	132.16
CAS:	104-55-2

Physical Properties

Property code	Value	Unit	Source

ea	0.82 ± 0.04	eV	NIST Webbook
gf	118.01	kJ/mol	Joback Method
hf	39.08	kJ/mol	Joback Method
hfus	15.60	kJ/mol	Joback Method
hvap	62.40	kJ/mol	NIST Webbook
log10ws	-1.99		Crippen Method
logp	1.899		Crippen Method
mcvol	111.180	ml/mol	McGowan Method
pc	3786.98	kPa	Joback Method
rinpol	1231.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1266.00		NIST Webbook
rinpol	1232.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1259.50		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1303.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1296.00		NIST Webbook
rinpol	1297.00		NIST Webbook
rinpol	1301.00		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1259.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1222.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1227.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1266.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1278.00		NIST Webbook
ripol	2013.20		NIST Webbook

ripol	1996.00		NIST Webbook
ripol	1996.00		NIST Webbook
ripol	1996.00		NIST Webbook
ripol	1986.00		NIST Webbook
ripol	2037.00		NIST Webbook
ripol	2039.00		NIST Webbook
ripol	2049.00		NIST Webbook
ripol	2029.00		NIST Webbook
ripol	2031.00		NIST Webbook
ripol	2019.00		NIST Webbook
ripol	2033.00		NIST Webbook
ripol	2034.00		NIST Webbook
ripol	2017.00		NIST Webbook
ripol	2017.00		NIST Webbook
ripol	2043.00		NIST Webbook
ripol	1978.00		NIST Webbook
ripol	2007.00		NIST Webbook
ripol	2007.00		NIST Webbook
ripol	2046.00		NIST Webbook
ripol	1996.00		NIST Webbook
ripol	2043.00		NIST Webbook
ripol	2018.00		NIST Webbook
ripol	2003.00		NIST Webbook
ripol	1996.00		NIST Webbook
ripol	2063.00		NIST Webbook
ripol	1996.00		NIST Webbook
tb	484.82	K	Joback Method
tc	708.10	K	Joback Method
tf	265.70 ± 0.70	K	NIST Webbook
vc	0.428	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.59	J/mol×K	484.82	Joback Method
cpg	229.63	J/mol×K	522.03	Joback Method
cpg	277.85	J/mol×K	708.10	Joback Method
cpg	269.63	J/mol×K	670.89	Joback Method
cpg	260.75	J/mol×K	633.68	Joback Method
cpg	251.16	J/mol×K	596.46	Joback Method
cpg	240.80	J/mol×K	559.25	Joback Method

dvisc	0.0026880	Pa×s	308.15	Density and Viscosity of Acrylonitrile + Cinnamaldehyde, + Anisaldehyde, and + Benzaldehyde at (298.15, 308.15, and 318.15) K
dvisc	0.0022960	Pa×s	318.15	Density and Viscosity of Acrylonitrile + Cinnamaldehyde, + Anisaldehyde, and + Benzaldehyde at (298.15, 308.15, and 318.15) K
dvisc	0.0034780	Pa×s	298.15	Density and Viscosity of Acrylonitrile + Cinnamaldehyde, + Anisaldehyde, and + Benzaldehyde at (298.15, 308.15, and 318.15) K
hvapt	72.70	kJ/mol	363.00	NIST Webbook
hvapt	58.20	kJ/mol	434.00	NIST Webbook
hvapt	51.70	kJ/mol	445.00	NIST Webbook
pvap	20.00	kPa	463.15	Isobaric vapor-liquid equilibrium for binary system of cinnamaldehyde + benzaldehyde at 10, 20 and 30 kPa
pvap	10.00	kPa	442.84	Isobaric vapor-liquid equilibrium for binary system of cinnamaldehyde + benzaldehyde at 10, 20 and 30 kPa
pvap	30.00	kPa	475.83	Isobaric vapor-liquid equilibrium for binary system of cinnamaldehyde + benzaldehyde at 10, 20 and 30 kPa

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Isobaric vapor-liquid equilibrium for binary system of cinnamaldehyde + benzaldehyde at 10, 20 and 30 kPa:	https://www.doi.org/10.1016/j.fluid.2013.12.002
Density and Viscosity of Acrylonitrile + Cinnamaldehyde, + Anisaldehyde, and + Benzaldehyde at (298.15, 308.15, and 318.15) K:	https://www.doi.org/10.1021/je7006742
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=C104552&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
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