3-Phenylpropanol

Other names:	(3-Hydroxypropyl)benzene
	1-Hydroxy-3-phenylpropane
	1-Propanol, 3-phenyl-
	3- Phenylprophyl alcohol
	3-Benzenepropanol
	3-Phenyl-1-propanol
	3-Phenyl-n-propanol
	3-Phenylpropan-1-ol
	3-Phenylpropyl alcohol
	3-phenyl-n-propyl alcohol
	Benzenepropanol
	Dihydrocinnamyl alcohol
	Hydrocinnamic alcohol
	Hydrocinnamyl alcohol
	NSC 16942
	Phenylpropyl alcohol
	Phenylpropylic alcohol
	propanol, 3-phenyl-
	«gamma»-Phenylpropanol
	«gamma»-Phenylpropyl alcohol
	Â«gammaÂ»-Phenylpropanol
	Â«gammaÂ»-Phenylpropyl alcohol
Inchi:	InChI=1S/C9H12O/c10-8-4-7-9-5-2-1-3-6-9/h1-3,5-6,10H,4,7-8H2
InchiKey:	VAJVDSVGBWFCLW-UHFFFAOYSA-N
Formula:	C9H12O
SMILES:	OCCCc1ccccc1
Mol. weight [g/mol]:	136.19
CAS:	122-97-4

Physical Properties

Property code	Value	Unit	Source
gf	0.49	kJ/mol	Joback Method
hf	-144.79	kJ/mol	Joback Method
hfus	17.20	kJ/mol	Joback Method
hvap	54.58	kJ/mol	Joback Method
log10ws	-1.38		Aqueous Solubility Prediction Method

logp	1.611		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3460.00	kPa	Vapor-Liquid Critical Properties of Phenol and (C8 to C10) Phenylalkanols
rinpol	1197.00		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1232.00		NIST Webbook
rinpol	1202.00		NIST Webbook
rinpol	1202.00		NIST Webbook
rinpol	1201.00		NIST Webbook
rinpol	1213.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1218.00		NIST Webbook
rinpol	1235.20		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1232.00		NIST Webbook
rinpol	1200.00		NIST Webbook
rinpol	1238.00		NIST Webbook
rinpol	1225.00		NIST Webbook
rinpol	1234.00		NIST Webbook
rinpol	1237.00		NIST Webbook
rinpol	1200.00		NIST Webbook
rinpol	1232.00		NIST Webbook
rinpol	1202.00		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1203.00		NIST Webbook
rinpol	1203.00		NIST Webbook
rinpol	1207.00		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1205.00		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1200.00		NIST Webbook
rinpol	1235.20		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1232.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1219.00		NIST Webbook
rinpol	1243.00		NIST Webbook
rinpol	1243.00		NIST Webbook
rinpol	1253.00		NIST Webbook
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ripol	1993.00		NIST Webbook

ripol	2037.00		NIST Webbook
ripol	2059.00		NIST Webbook
ripol	2040.00		NIST Webbook
ripol	2039.00		NIST Webbook
ripol	1993.00		NIST Webbook
ripol	2049.00		NIST Webbook
ripol	1989.00		NIST Webbook
ripol	2045.00		NIST Webbook
ripol	2047.00		NIST Webbook
ripol	2045.00		NIST Webbook
ripol	2058.00		NIST Webbook
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ripol	2032.00		NIST Webbook
ripol	2007.00		NIST Webbook
ripol	2022.00		NIST Webbook
ripol	2037.00		NIST Webbook
ripol	2016.00		NIST Webbook
ripol	2036.00		NIST Webbook
ripol	2058.00		NIST Webbook
ripol	2061.00		NIST Webbook
ripol	1989.00		NIST Webbook
ripol	2049.00		NIST Webbook
tb	508.20	K	NIST Webbook
tb	515.15 ± 0.40	K	NIST Webbook
tb	486.00 ± 2.00	K	NIST Webbook
tc	719.09	K	Joback Method
tf	278.43	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.76	J/mol×K	686.60	Joback Method
cpg	266.71	J/mol×K	524.18	Joback Method
cpg	278.37	J/mol×K	556.66	Joback Method
cpg	289.37	J/mol×K	589.15	Joback Method
cpg	299.75	J/mol×K	621.63	Joback Method
cpg	309.54	J/mol×K	654.12	Joback Method
cpg	327.43	J/mol×K	719.09	Joback Method
cpl	280.74	J/mol×K	298.15	NIST Webbook

dvisc	0.0001251	Pa×s	524.18	Joback Method
dvisc	0.0168187	Pa×s	278.43	Joback Method
dvisc	0.0044008	Pa×s	319.39	Joback Method
dvisc	0.0015618	Pa×s	360.35	Joback Method
dvisc	0.0006848	Pa×s	401.30	Joback Method
dvisc	0.0003498	Pa×s	442.26	Joback Method
dvisc	0.0002002	Pa×s	483.22	Joback Method
hvapt	62.60	kJ/mol	427.50	NIST Webbook
hvapt	62.80	kJ/mol	306.00	NIST Webbook
rfi	1.52100		308.15	Excess Enthalpies, Heat Capacities, Densities, Viscosities and Refractive Indices of Dimethyl Sulfoxide + Three Aryl Alcohols at 308.15 K and Atmospheric Pressure
rfi	1.52590		298.15	Enthalpies of Mixing, Densities, and Refractive Indices for Binary Mixtures of (Anisole or Phenetole) + Three Aryl Alcohols at 308.15 K and at Atmospheric Pressure
rfi	1.52140		308.15	Enthalpies of Mixing, Densities, and Refractive Indices for Binary Mixtures of (Anisole or Phenetole) + Three Aryl Alcohols at 308.15 K and at Atmospheric Pressure
rhol	990.81	kg/m3	308.15	Excess Properties of Binary Mixtures of Esters of Carbonic Acid + Three Aryl Alcohols at 308.15 K

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	392.20	K	1.60	NIST Webbook

Sources

Enthalpies of Mixing, Densities, and Refractive Indices for Binary Mixtures of Anisole or Phenetole + Three Aryl Alcohols at 308.15 K and at Atmospheric Pressure:	https://www.doi.org/10.1021/je050085p
Excess Enthalpies, Heat Capacities, Densities, Viscosities, and Refractive Indices for Binary Mixtures of Anisole or Phenetole + Three Aryl Alcohols at 308.15 K and at Atmospheric Pressure:	https://www.doi.org/10.1021/je0501991
Vapor-Liquid Critical Properties of Phenol and (C1 to C10) Phenylalkanols: NIST Webbook:	https://www.doi.org/10.1021/je0604380
Vapor-Liquid Critical Properties of Phenol and (C1 to C10) Phenylalkanols: NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C122974&Units=SI
Excess Properties of Binary Mixtures of Esters of Carbonic Acid + Three Aryl Alcohols at 308.15 K:	https://www.doi.org/10.1021/je0497395
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Partitioning of Phenylalkanols between Micelles and Water Studied by Limiting Interdiffusion Coefficients in Water and Tetradecyltrimethylammonium Bromide Solutions:	https://www.doi.org/10.1021/je900967j
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
rfi:	Refractive Index
rhol:	Liquid Density
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

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