Benzene, ethoxy-

Other names:	Benzyl methyl ether
	ETHOXYBENZENE
	ETHYL PHENYL ETHER
	Ether, ethyl phenyl-
	PHENOXYETHANE
	Phenetole
	Phenyl ethyl ether
Inchi:	InChI=1S/C8H10O/c1-2-9-8-6-4-3-5-7-8/h3-7H,2H2,1H3
InchiKey:	DLRJIFUOBPOJNS-UHFFFAOYSA-N
Formula:	C8H10O
SMILES:	CCOc1ccccc1
Mol. weight [g/mol]:	122.16
CAS:	103-73-1

Physical Properties

Property code	Value	Unit	Source
af	0.4180		KDB
chl	-4424.59	kJ/mol	NIST Webbook
chl	-4417.84	kJ/mol	NIST Webbook
dm	1.20	debye	KDB
gf	23.89	kJ/mol	Joback Method
hf	-101.60 ± 1.20	kJ/mol	NIST Webbook
hf	-108.40	kJ/mol	NIST Webbook
hf	-125.00	kJ/mol	NIST Webbook
hfl	-152.60 ± 1.20	kJ/mol	NIST Webbook
hfl	-159.40	kJ/mol	NIST Webbook
hfus	11.70	kJ/mol	Joback Method
hvap	51.00 ± 0.10	kJ/mol	NIST Webbook
hvap	51.00	kJ/mol	NIST Webbook
hvap	50.70	kJ/mol	NIST Webbook
hvap	51.04	kJ/mol	NIST Webbook
hvap	51.04 ± 0.12	kJ/mol	NIST Webbook
ie	8.13 ± 0.02	eV	NIST Webbook
ie	8.36	eV	NIST Webbook
ie	8.41	eV	NIST Webbook
ie	8.60	eV	NIST Webbook

log10ws	-2.33		Aqueous Solubility Prediction Method
log10ws	-2.33		Estimated Solubility Method
logp	2.085		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
pc	3434.92 ± 101.32	kPa	NIST Webbook
pc	3414.65 ± 101.32	kPa	NIST Webbook
pc	3420.00	kPa	KDB
pc	3420.00 ± 81.06	kPa	NIST Webbook
rinpol	988.80		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	953.70		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	991.10		NIST Webbook
rinpol	992.40		NIST Webbook
rinpol	970.80		NIST Webbook
rinpol	988.80		NIST Webbook
rinpol	991.10		NIST Webbook
rinpol	992.40		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	978.10		NIST Webbook
rinpol	980.50		NIST Webbook
rinpol	973.30		NIST Webbook
rinpol	971.60		NIST Webbook
rinpol	981.30		NIST Webbook
rinpol	976.30		NIST Webbook
rinpol	978.50		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	996.00		NIST Webbook
ripol	1442.00		NIST Webbook
ripol	1437.00		NIST Webbook
tb	442.96	K	KDB
tc	647.00	K	KDB
tc	647.15 ± 2.50	K	NIST Webbook
tc	647.00 ± 2.00	K	NIST Webbook
tf	243.48 ± 0.30	K	NIST Webbook
tf	243.68 ± 0.30	K	NIST Webbook
tf	243.63 ± 0.05	K	NIST Webbook
tf	243.32	K	Aqueous Solubility Prediction Method
tf	243.63	K	KDB

tf	242.95 ± 0.30	K	NIST Webbook
vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.55	J/mol×K	466.27	Joback Method
cpg	263.60	J/mol×K	639.91	Joback Method
cpg	254.14	J/mol×K	605.18	Joback Method
cpg	244.12	J/mol×K	570.45	Joback Method
cpg	233.52	J/mol×K	535.73	Joback Method
cpg	222.34	J/mol×K	501.00	Joback Method
cpg	198.15	J/mol×K	431.54	Joback Method
cpl	228.50	J/mol×K	298.15	NIST Webbook
dvisc	0.0012913	Pa×s	262.40	Joback Method
dvisc	0.0007596	Pa×s	296.23	Joback Method
dvisc	0.0004982	Pa×s	330.06	Joback Method
dvisc	0.0003534	Pa×s	363.88	Joback Method
dvisc	0.0002657	Pa×s	397.71	Joback Method
dvisc	0.0002090	Pa×s	431.54	Joback Method
dvisc	0.0025685	Pa×s	228.57	Joback Method
hvapt	44.50	kJ/mol	422.00	NIST Webbook
hvapt	40.70	kJ/mol	422.00	NIST Webbook
hvapt	44.00	kJ/mol	427.00	NIST Webbook
rfi	1.50020		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
rfi	1.50580		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

rhol	951.00	kg/m3	308.00	Densities, ultrasonic speeds and refractive indices of phenetole with N-methyl-2-pyrrolidone, N,N-dimethylformamide and tetrahydrofuran binary mixtures at different temperatures
rhol	942.50	kg/m3	318.15	Intermolecular interactions in mixtures of poly (ethylene glycol) with methoxybenzene and ethoxybenzene: Volumetric and viscometric studies
rhol	953.40	kg/m3	308.15	Intermolecular interactions in mixtures of poly (ethylene glycol) with methoxybenzene and ethoxybenzene: Volumetric and viscometric studies
rhol	960.20	kg/m3	298.15	Intermolecular interactions in mixtures of poly (ethylene glycol) with methoxybenzene and ethoxybenzene: Volumetric and viscometric studies
rhol	979.00	kg/m3	277.00	KDB
rhol	955.00	kg/m3	303.00	Densities, ultrasonic speeds and refractive indices of phenetole with N-methyl-2-pyrrolidone, N,N-dimethylformamide and tetrahydrofuran binary mixtures at different temperatures

rhol	960.00	kg/m3	298.00	Densities, ultrasonic speeds and refractive indices of phenetole with N-methyl-2-pyrrolidone, N,N-dimethylformamide and tetrahydrofuran binary mixtures at different temperatures

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	333.20	K	1.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47771e+01
Coeff. B	-3.92315e+03
Coeff. C	-5.72150e+01
Temperature range (K), min.	327.97
Temperature range (K), max.	471.68

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.30608e+01
Coeff. B	-9.14632e+03
Coeff. C	-1.13117e+01
Coeff. D	5.75060e-06
Temperature range (K), min.	243.63
Temperature range (K), max.	647.15

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103731&Units=SI
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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1028.mol
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1028
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Intermolecular interactions in mixtures of poly (ethylene glycol) with methoxybenzene and ethoxybenzene:	https://www.doi.org/10.1016/j.jct.2013.12.008
Densities, ultrasonic speeds and refractive indices of phenetole with 1-alkanols at 298.15 K:	https://www.doi.org/10.1016/j.jct.2016.07.032
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Volumetric and isentropic studies of N-methyl-2-pyrrolidone (1) + N,N-dimethylformamide and tetrahydrofuran binary mixtures at different temperatures:	

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor 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