Ethanol, 2-phenoxy-

Other names:	.beta.-phenoxyethyl alcohol
	1-Hydroxy-2-phenoxyethane
	2-Fenoxyethanol
	2-Hydroxyethyl phenyl ether
	2-Phenoxyethanol
	2-Phenoxyethanol (rose ether)
	2-Phenoxyethyl alcohol
	Arosol
	Dowanol EP
	Dowanol eph
	Emeressence 1160
	Emery 6705
	Ethylene glycol monophenyl ether
	Ethylene glycol phenyl ether
	Fenyl-cellosolve
	Fenylcelosolv
	Glycol monophenyl ether
	NSC 1864
	Phenoxethol
	Phenoxetol
	Phenoxyethanol
	Phenoxyethyl alcohol
	Phenoxyl ethanol
	Phenoxytol
	Phenyl cellosolve
	Phenylmonoglycol ether
	Rose ether
	«beta»-Hydroxyethyl phenyl ether
	«beta»-Phenoxyethanol
	«beta»-Phenoxyethyl alcohol
	Â«betaÂ»-Hydroxyethyl phenyl ether
	Â«betaÂ»-Phenoxyethanol
	Â«betaÂ»-Phenoxyethyl alcohol
Inchi:	InChI=1S/C8H10O2/c9-6-7-10-8-4-2-1-3-5-8/h1-5,9H,6-7H2
InchiKey:	QCDWFXQBSFUVSP-UHFFFAOYSA-N
Formula:	C8H10O2
SMILES:	OCCOc1ccccc1
Mol. weight [g/mol]:	138.16
CAS:	122-99-6

Physical Properties

Property code	Value	Unit	Source
gf	-112.93	kJ/mol	Joback Method
hf	-256.37	kJ/mol	Joback Method
hfus	15.79	kJ/mol	Joback Method
hvap	54.77	kJ/mol	Joback Method
log10ws	-0.70		Estimated Solubility Method
log10ws	-0.70		Aqueous Solubility Prediction Method
logp	1.058		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
pc	4005.77	kPa	Joback Method
rinpol	1191.60		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1210.00		NIST Webbook
rinpol	1214.00		NIST Webbook
rinpol	1191.60		NIST Webbook
rinpol	1186.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1226.00		NIST Webbook
rinpol	1245.30		NIST Webbook
rinpol	1229.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1226.00		NIST Webbook
rinpol	1226.00		NIST Webbook
rinpol	1189.00		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1213.00		NIST Webbook
ripol	2100.00		NIST Webbook
ripol	2103.00		NIST Webbook
ripol	2115.00		NIST Webbook
ripol	2139.00		NIST Webbook
ripol	2103.00		NIST Webbook
ripol	2087.00		NIST Webbook
ripol	2144.00		NIST Webbook

ripol	2126.00		NIST Webbook
ripol	2142.00		NIST Webbook
ripol	2107.00		NIST Webbook
ripol	2080.00		NIST Webbook
ripol	2115.00		NIST Webbook
tb	510.20	K	NIST Webbook
tb	518.20	K	NIST Webbook
tc	719.69	K	Joback Method
tf	285.90	K	Aqueous Solubility Prediction Method
vc	0.412	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.88	J/mol×K	523.72	Joback Method
cpg	256.37	J/mol×K	556.38	Joback Method
cpg	266.32	J/mol×K	589.04	Joback Method
cpg	275.73	J/mol×K	621.70	Joback Method
cpg	284.64	J/mol×K	654.37	Joback Method
cpg	293.04	J/mol×K	687.03	Joback Method
cpg	300.95	J/mol×K	719.69	Joback Method
cpl	294.63	J/mol×K	298.15	NIST Webbook
dvisc	0.0001115	Pa×s	523.72	Joback Method
dvisc	0.0031358	Pa×s	328.44	Joback Method
dvisc	0.0012117	Pa×s	367.50	Joback Method
dvisc	0.0104901	Pa×s	289.39	Joback Method
dvisc	0.0002983	Pa×s	445.61	Joback Method
dvisc	0.0001753	Pa×s	484.67	Joback Method
dvisc	0.0005620	Pa×s	406.56	Joback Method
hvapt	66.00	kJ/mol	435.00	NIST Webbook
rhol	1107.00	kg/m3	293.15	Density, speed of sound and refractive index of mixtures containing 2-phenoxyethanol with propanol or butanol at various temperatures

rhol	1099.00	kg/m3	303.15	Density, speed of sound and refractive index of mixtures containing 2-phenoxyethanol with propanol or butanol at various temperatures
rhol	1090.00	kg/m3	313.15	Density, speed of sound and refractive index of mixtures containing 2-phenoxyethanol with propanol or butanol at various temperatures
rhol	1081.00	kg/m3	323.15	Density, speed of sound and refractive index of mixtures containing 2-phenoxyethanol with propanol or butanol at various temperatures
rhol	1103.00	kg/m3	298.15	Density, speed of sound and refractive index of mixtures containing 2-phenoxyethanol with propanol or butanol at various temperatures
rhol	1103.41	kg/m3	298.15	THERMODYNAMICS OF MIXTURES CONTAINING ALKOXYETHANOLS. XXVIII. LIQUID-LIQUID EQUILIBRIA FOR 2-PHENOXYETHANOL + SELECTED ALKANES

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55600e+01
Coeff. B	-4.77760e+03
Coeff. C	-8.15080e+01
Temperature range (K), min.	394.33
Temperature range (K), max.	547.68

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
THERMODYNAMICS OF MIXTURES CONTAINING ALKOXYETHANOLS. XXVII. LIQUID-LIQUID EQUILIBRIA FOR 2-PHENOXYETHANOL + SELECTED ALKANES:	https://www.doi.org/10.1016/j.tca.2011.04.012
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C122996&Units=SI
Density, speed of sound and refractive index of mixtures containing 2-phenoxyethanol with propanol or butanol at various temperatures:	https://www.doi.org/10.1016/j.jct.2018.08.029

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
pvap:	Vapor pressure
rhol:	Liquid Density
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