Benzoic acid, 2-ethylhexyl ester

Other names: 2-Ethyl-1-hexanol benzoate
2-ethylhexyl benzoate
Ethylhexyl benzoate
Inchi: InChI=1S/C15H22O2/c1-3-5-9-13(4-2)12-17-15(16)14-10-7-6-8-11-14/h6-8,10-11,13H,3-
InchiKey: UADWUILHKRXHMM-UHFFFAOYSA-N
Formula: C15H22O3
SMILES: CCCCC(CC)COC(=O)c1ccccc1
Mol. weight [g/mol]: 250.33
CAS: 5444-75-7

Physical Properties

Property code	Value	Unit	Source
gf	-48.53	kJ/mol	Joback Method
hf	-366.48	kJ/mol	Joback Method
hfus	27.91	kJ/mol	Joback Method
hvap	60.03	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.060		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	1935.54	kPa	Joback Method
rinpol	1735.00		NIST Webbook
rinpol	1674.00		NIST Webbook
rinpol	1735.00		NIST Webbook
rinpol	1674.00		NIST Webbook
ripol	2598.00		NIST Webbook
ripol	2598.00		NIST Webbook
tb	645.13	K	Joback Method
tc	846.21	K	Joback Method
tf	342.39	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	635.49	J/mol×K	846.21	Joback Method
cpg	546.83	J/mol×K	645.13	Joback Method
cpg	580.10	J/mol×K	712.16	Joback Method
cpg	595.30	J/mol×K	745.67	Joback Method
cpg	609.57	J/mol×K	779.18	Joback Method
cpg	622.96	J/mol×K	812.70	Joback Method
cpg	563.95	J/mol×K	678.64	Joback Method
dvisc	0.0024547	Pa×s	342.39	Joback Method
dvisc	0.0003541	Pa×s	493.76	Joback Method
dvisc	0.0010907	Pa×s	392.85	Joback Method
dvisc	0.0005830	Pa×s	443.30	Joback Method
dvisc	0.0002360	Pa×s	544.22	Joback Method
dvisc	0.0001684	Pa×s	594.67	Joback Method
dvisc	0.0001267	Pa×s	645.13	Joback Method
rhol	981.12	kg/m3	273.15	Temperature and Pressure Dependence of the Viscosities of 2-Ethylhexyl Benzoate, Bis(2-ethylhexyl) Phthalate, 2,6,10,15,19,23-Hexamethyltetracosane (Squalane), and Diisodecyl Phthalate
rhol	977.18	kg/m3	278.15	Temperature and Pressure Dependence of the Viscosities of 2-Ethylhexyl Benzoate, Bis(2-ethylhexyl) Phthalate, 2,6,10,15,19,23-Hexamethyltetracosane (Squalane), and Diisodecyl Phthalate
rhol	910.61	kg/m3	363.15	Temperature and Pressure Dependence of the Viscosities of 2-Ethylhexyl Benzoate, Bis(2-ethylhexyl) Phthalate, 2,6,10,15,19,23-Hexamethyltetracosane (Squalane), and Diisodecyl Phthalate

rhol	973.25	kg/m3	283.15	Temperature and Pressure Dependence of the Viscosities of 2-Ethylhexyl Benzoate, Bis(2-ethylhexyl) Phthalate, 2,6,10,15,19,23-Hexamethyltetracosane (Squalane), and Diisodecyl Phthalate
rhol	969.32	kg/m3	288.15	Temperature and Pressure Dependence of the Viscosities of 2-Ethylhexyl Benzoate, Bis(2-ethylhexyl) Phthalate, 2,6,10,15,19,23-Hexamethyltetracosane (Squalane), and Diisodecyl Phthalate
rhol	961.49	kg/m3	298.15	Temperature and Pressure Dependence of the Viscosities of 2-Ethylhexyl Benzoate, Bis(2-ethylhexyl) Phthalate, 2,6,10,15,19,23-Hexamethyltetracosane (Squalane), and Diisodecyl Phthalate
rhol	957.57	kg/m3	303.15	Temperature and Pressure Dependence of the Viscosities of 2-Ethylhexyl Benzoate, Bis(2-ethylhexyl) Phthalate, 2,6,10,15,19,23-Hexamethyltetracosane (Squalane), and Diisodecyl Phthalate
rhol	949.73	kg/m3	313.15	Temperature and Pressure Dependence of the Viscosities of 2-Ethylhexyl Benzoate, Bis(2-ethylhexyl) Phthalate, 2,6,10,15,19,23-Hexamethyltetracosane (Squalane), and Diisodecyl Phthalate

rhol	941.92	kg/m3	323.15	Temperature and Pressure Dependence of the Viscosities of 2-Ethylhexyl Benzoate, Bis(2-ethylhexyl) Phthalate, 2,6,10,15,19,23-Hexamethyltetracosane (Squalane), and Diisodecyl Phthalate
rhol	934.11	kg/m3	333.15	Temperature and Pressure Dependence of the Viscosities of 2-Ethylhexyl Benzoate, Bis(2-ethylhexyl) Phthalate, 2,6,10,15,19,23-Hexamethyltetracosane (Squalane), and Diisodecyl Phthalate
rhol	926.28	kg/m3	343.15	Temperature and Pressure Dependence of the Viscosities of 2-Ethylhexyl Benzoate, Bis(2-ethylhexyl) Phthalate, 2,6,10,15,19,23-Hexamethyltetracosane (Squalane), and Diisodecyl Phthalate
rhol	918.45	kg/m3	353.15	Temperature and Pressure Dependence of the Viscosities of 2-Ethylhexyl Benzoate, Bis(2-ethylhexyl) Phthalate, 2,6,10,15,19,23-Hexamethyltetracosane (Squalane), and Diisodecyl Phthalate
rhol	965.40	kg/m3	293.15	Temperature and Pressure Dependence of the Viscosities of 2-Ethylhexyl Benzoate, Bis(2-ethylhexyl) Phthalate, 2,6,10,15,19,23-Hexamethyltetracosane (Squalane), and Diisodecyl Phthalate

sdco	2.54e-04	m2/s	313.06	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	2.92e-04	m2/s	318.06	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	3.74e-04	m2/s	327.81	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	3.74e-04	m2/s	327.87	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	4.18e-04	m2/s	332.77	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	4.18e-04	m2/s	332.80	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	4.22e-04	m2/s	333.30	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	2.91e-04	m2/s	317.99	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	4.71e-04	m2/s	337.81	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	5.84e-04	m2/s	347.49	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	5.82e-04	m2/s	347.52	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	6.38e-04	m2/s	352.18	Viscous Calibration Liquids for Self-diffusion Measurements

sdco	6.36e-04	m2/s	352.33	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	6.36e-04	m2/s	352.41	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	2.54e-04	m2/s	313.05	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	4.72e-04	m2/s	337.81	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	2.21e-04	m2/s	308.30	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	2.22e-04	m2/s	308.26	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	2.26e-04	m2/s	308.07	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	2.25e-04	m2/s	307.92	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	1.60e-04	m2/s	298.29	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	1.60e-04	m2/s	298.27	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	1.65e-04	m2/s	298.14	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	1.64e-04	m2/s	298.09	Viscous Calibration Liquids for Self-diffusion Measurements

sdco	1.63e-04	m2/s	298.06	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	1.35e-04	m2/s	293.38	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	1.34e-04	m2/s	293.37	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	1.11e-04	m2/s	288.46	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	1.10e-04	m2/s	288.41	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	7.33e-05	m2/s	278.50	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	7.27e-05	m2/s	278.45	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	7.24e-05	m2/s	278.43	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	7.32e-05	m2/s	278.40	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	5.67e-05	m2/s	273.67	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	5.61e-05	m2/s	273.50	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	5.57e-05	m2/s	273.42	Viscous Calibration Liquids for Self-diffusion Measurements

sdco	3.31e-05	m2/s	264.21	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	3.30e-05	m2/s	264.21	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	2.21e-05	m2/s	258.46	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	2.18e-05	m2/s	258.44	Viscous Calibration Liquids for Self-diffusion Measurements
sdco	2.26e-05	m2/s	258.42	Viscous Calibration Liquids for Self-diffusion Measurements

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Viscous Calibration Liquids for Self-diffusion Measurements:	https://www.doi.org/10.1021/acs.jced.5b00246
Temperature and Pressure Dependence of the Viscosities of 2-Ethylhexyl Benzoate, Bis(2-ethylhexyl) Phthalate, 2,6,10,15,19,23-Hexamethyltetracosane (Squalane), and Diisodecyl Phthalate:	https://www.doi.org/10.1021/je900284z
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=C5444757&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
log10ws:	Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sdco:	Self diffusion coefficient
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume