Butane, 1-(ethenyloxy)-

Other names:	1-(ETHYNYLOXY)BUTANE
	1-(Ethenyloxy)butane
	1-(Vinyloxy)-butane
	1-(vinyloxy)butane
	1-Butoxyethylene
	1-vinyloxybutane
	BUTOXYETHENE
	BVE
	Butoxyethylene
	Butyl vinyl ether
	Ethenyl n-butyl ether
	Ether, butyl vinyl
	NSC 8264
	VINYL N-BUTYL ETHER
	Vinyl butyl ether
	n-Butyl vinyl ether
	n-C4H9OCH=CH2
Inchi:	InChI=1S/C6H12O/c1-3-5-6-7-4-2/h4H,2-3,5-6H2,1H3
InchiKey:	UZKWTJUDCOPSNM-UHFFFAOYSA-N
Formula:	C6H12O
SMILES:	C=COCCCC
Mol. weight [g/mol]:	100.16
CAS:	111-34-2

Physical Properties

Property code	Value	Unit	Source
chl	-3860.20 ± 1.10	kJ/mol	NIST Webbook
chl	-3857.00 ± 0.80	kJ/mol	NIST Webbook
gf	-17.52	kJ/mol	Joback Method
hf	-179.20 ± 1.20	kJ/mol	NIST Webbook
hf	-182.40	kJ/mol	NIST Webbook
hfl	-219.00 ± 0.80	kJ/mol	NIST Webbook
hfl	-215.80 ± 1.20	kJ/mol	NIST Webbook
hfus	11.20	kJ/mol	Joback Method
hvap	30.69	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.947		Crippen Method

mcvol	96.970	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
nfpas	%!d(float64=2)		KDB
pc	3200.00 ± 250.00	kPa	NIST Webbook
rhoc	261.11 ± 12.02	kg/m3	NIST Webbook
rinpol	695.00		NIST Webbook
rinpol	671.00		NIST Webbook
rinpol	679.00		NIST Webbook
rinpol	687.00		NIST Webbook
rinpol	695.00		NIST Webbook
ripol	858.00		NIST Webbook
tb	367.10	K	NIST Webbook
tb	366.00	K	NIST Webbook
tb	367.00	K	NIST Webbook
tc	540.50 ± 2.00	K	NIST Webbook
tf	177.85	K	Joback Method
vc	0.370	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.18	J/mol×K	411.75	Joback Method
cpg	168.37	J/mol×K	355.78	Joback Method
cpg	196.15	J/mol×K	439.73	Joback Method
cpg	204.82	J/mol×K	467.71	Joback Method
cpg	213.21	J/mol×K	495.69	Joback Method
cpg	221.32	J/mol×K	523.68	Joback Method
cpg	177.92	J/mol×K	383.76	Joback Method
cpl	231.80	J/mol×K	298.15	NIST Webbook
dvisc	0.0013807	Pa×s	207.51	Joback Method
dvisc	0.0007872	Pa×s	237.16	Joback Method
dvisc	0.0005086	Pa×s	266.81	Joback Method
dvisc	0.0003585	Pa×s	296.47	Joback Method
dvisc	0.0002694	Pa×s	326.12	Joback Method
dvisc	0.0029205	Pa×s	177.85	Joback Method
dvisc	0.0002123	Pa×s	355.78	Joback Method
hvapt	36.10	kJ/mol	318.50	NIST Webbook
hvapt	29.60 ± 0.20	kJ/mol	357.00	NIST Webbook
hvapt	32.50 ± 0.20	kJ/mol	357.00	NIST Webbook
hvapt	35.20 ± 0.20	kJ/mol	357.00	NIST Webbook

hvapt	31.58	kJ/mol	367.10	NIST Webbook
rhol	763.30	kg/m3	313.15	Densities, Viscosities, and Sound Speed of Binary Mixtures of Hexyl Acetate with Tetrahydrofuran, 1,4-Dioxane, Anisole, and Butyl Vinyl Ether
rhol	769.00	kg/m3	303.15	Density, viscosity, and speed of sound of binary liquid mixtures of vinyl acetate with butyl vinyl ether, diisopropyl ether, anisole and dibutyl ether
rhol	768.20	kg/m3	308.15	Densities, Viscosities, and Sound Speed of Binary Mixtures of Hexyl Acetate with Tetrahydrofuran, 1,4-Dioxane, Anisole, and Butyl Vinyl Ether
rhol	774.10	kg/m3	303.15	Densities, Viscosities, and Sound Speed of Binary Mixtures of Hexyl Acetate with Tetrahydrofuran, 1,4-Dioxane, Anisole, and Butyl Vinyl Ether
rhol	780.20	kg/m3	298.15	Densities, Viscosities, and Sound Speed of Binary Mixtures of Hexyl Acetate with Tetrahydrofuran, 1,4-Dioxane, Anisole, and Butyl Vinyl Ether
rhol	758.80	kg/m3	313.15	Density, viscosity, and speed of sound of binary liquid mixtures of vinyl acetate with butyl vinyl ether, diisopropyl ether, anisole and dibutyl ether

rhol	763.90	kg/m3	308.15	Density, viscosity, and speed of sound of binary liquid mixtures of vinyl acetate with butyl vinyl ether, diisopropyl ether, anisole and dibutyl ether

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54615e+01
Coeff. B	-3.51136e+03
Coeff. C	-4.31680e+01
Temperature range (K), min.	274.58
Temperature range (K), max.	389.11

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.18610e+01
Coeff. B	-7.10617e+03
Coeff. C	-9.96430e+00
Coeff. D	7.13053e-06
Temperature range (K), min.	181.15
Temperature range (K), max.	536.00

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1012
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Densities, Viscosities, and Sound Speed of Binary Mixtures of Hexyl Acetate with Tetrahydrofuran, 1,4-Dioxane, Anisole, and Butyl Vinyl Ether:	https://www.doi.org/10.1021/je400539h
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111342&Units=SI

Density, viscosity, and speed of sound of binary liquid mixtures of vinyl acetate with butyl vinyl ether, diisopropyl ether, anisole and dibutyl ether:	https://www.doi.org/10.1016/j.jct.2019.04.018
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1012.mol
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
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
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
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