Butane, 1,1'-[ethylidenebis(oxy)]bis-

Other names:	1,1'-[ethylidenebis(oxy)]dibutane
	1,1-DIBUTOXYETHANE
	1,1-Di-n-butoxyethane
	6-METHYL-5,7-DIOXAUNDECANE
	Acetaldehyde, dibutyl acetal
	DIBUTYL ACETAL ACETALDEHYDE
	Di-n-butyl acetal
	Dibutyl acetal
	Ethane, 1,1-dibutoxy-
Inchi:	InChI=1S/C10H22O2/c1-4-6-8-11-10(3)12-9-7-5-2/h10H,4-9H2,1-3H3
InchiKey:	SWTCCCJQNPGXLQ-UHFFFAOYSA-N
Formula:	C10H22O2
SMILES:	CCCCOC(C)OCCCC
Mol. weight [g/mol]:	174.28
CAS:	871-22-7

Physical Properties

Property code	Value	Unit	Source
gf	-179.12	kJ/mol	Joback Method
hf	-519.45	kJ/mol	Joback Method
hfus	20.51	kJ/mol	Joback Method
hvap	42.29	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.966		Crippen Method
mcvol	163.500	ml/mol	McGowan Method
pc	2058.62	kPa	Joback Method
rinpol	1095.00		NIST Webbook
tb	459.00 ± 4.00	K	NIST Webbook
tb	371.85 ± 0.50	K	NIST Webbook
tc	638.49	K	Joback Method
tf	231.92	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.18	J/mol×K	610.84	Joback Method
cpg	369.40	J/mol×K	472.60	Joback Method
cpg	384.29	J/mol×K	500.25	Joback Method
cpg	398.71	J/mol×K	527.90	Joback Method
cpg	412.67	J/mol×K	555.54	Joback Method
cpg	426.16	J/mol×K	583.19	Joback Method
cpg	451.74	J/mol×K	638.49	Joback Method
cpl	352.20	J/mol×K	298.00	NIST Webbook
dvisc	0.0001614	Pa×s	472.60	Joback Method
dvisc	0.0046878	Pa×s	231.92	Joback Method
dvisc	0.0017676	Pa×s	272.03	Joback Method
dvisc	0.0008564	Pa×s	312.15	Joback Method
dvisc	0.0004893	Pa×s	352.26	Joback Method
dvisc	0.0003135	Pa×s	392.37	Joback Method
dvisc	0.0002182	Pa×s	432.49	Joback Method
hvapt	47.30	kJ/mol	383.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.21214e+01
Coeff. B	-8.38283e+03
Coeff. C	-8.22314e+00
Coeff. D	5.20306e-06
Temperature range (K), min.	303.15
Temperature range (K), max.	461.15

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1052

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1052.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C871227&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume