Di-sec-Butyl ether

Other names:	(sec-C4H9)2O
	2,2'-OXYBIS-BUTANE
	2,2'-Oxybisbutane
	3,5-dimethyl-4-oxaheptane
	Bis(2-butyl)ether
	Butane, 2,2'-oxybis-
	SEC-BUTYL ETHER
	bis(2-butyl) ether
	bis-(1-methylpropyl) ether
Inchi:	InChI=1S/C8H18O/c1-5-7(3)9-8(4)6-2/h7-8H,5-6H2,1-4H3
InchiKey:	HHBZZTKMMLDNDN-UHFFFAOYSA-N
Formula:	C8H18O
SMILES:	CCC(C)OC(C)CC
Mol. weight [g/mol]:	130.23
CAS:	6863-58-7

Physical Properties

Property code	Value	Unit	Source
af	0.4100		KDB
affp	865.90	kJ/mol	NIST Webbook
basg	838.50	kJ/mol	NIST Webbook
chl	-5319.00 ± 1.00	kJ/mol	NIST Webbook
gf	-93.40	kJ/mol	Joback Method
hf	-361.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-401.60 ± 1.10	kJ/mol	NIST Webbook
hfus	10.62	kJ/mol	Joback Method
hvap	40.88	kJ/mol	NIST Webbook
ie	9.11	eV	NIST Webbook
log10ws	-2.48		Crippen Method
logp	2.600		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2550.00	kPa	KDB
tb	394.20	K	KDB
tb	394.00	K	NIST Webbook
tb	394.20	K	NIST Webbook
tc	562.00	K	KDB
tf	172.00	K	KDB

vc	0.489	m3/kmol	KDB
zc	0.2671280		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.51	J/mol×K	575.40	Joback Method
cpg	320.23	J/mol×K	546.83	Joback Method
cpg	308.52	J/mol×K	518.26	Joback Method
cpg	296.39	J/mol×K	489.69	Joback Method
cpg	283.82	J/mol×K	461.12	Joback Method
cpg	270.82	J/mol×K	432.55	Joback Method
cpg	257.37	J/mol×K	403.98	Joback Method
dvisc	0.0136903	Pa×s	172.15	Joback Method
dvisc	0.0002043	Pa×s	403.98	Joback Method
dvisc	0.0002842	Pa×s	365.34	Joback Method
dvisc	0.0004275	Pa×s	326.70	Joback Method
dvisc	0.0007176	Pa×s	288.06	Joback Method
dvisc	0.0014141	Pa×s	249.43	Joback Method
dvisc	0.0035734	Pa×s	210.79	Joback Method
hvapt	34.06	kJ/mol	394.20	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54197e+01
Coeff. B	-3.70770e+03
Coeff. C	-5.07380e+01
Temperature range (K), min.	295.76
Temperature range (K), max.	417.54

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.78094e+01

Coeff. B	-7.85694e+03
Coeff. C	-1.07579e+01
Coeff. D	6.67024e-06
Temperature range (K), min.	173.15
Temperature range (K), max.	559.00

Sources

KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1021
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6863587&Units=SI
Liquid liquid equilibria for binary systems of tert-amyl ethyl ether (TAEE), isopropyl tert-butyl ether (IPTBE) and di-sec-butyl ether (DSBE) with water and for ternary systems with methanol or ethanol:	https://www.doi.org/10.1016/j.fluid.2007.04.018
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1021
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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
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

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility